STIC Search Report
Biotech-Chem Library

STIC Database Tracking Number: 181023

TO:	From:
Marcela Cordero Garcia **Location: rem/3c35/3c18** **Art Unit: 1654** **Wednesday, March 01, 2006** **Case Serial Number: 10/822639**	**John DiNatale** **Location: Biotech-Chem Library** **REM-1B65** **Phone: (571)272-2557** **john.dinatale@uspto.gov**

Search Notes

Examiner Cordero Garcia,

See attached results.

If you have any questions about this search feel free to contact me at any time.

Thank you for using STIC search services!

John DiNatale
Technical Information Specialist
STIC Biotech/Chem Library
(571)272-2557

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ACCESS DB # _____

PLEASE PRINT CLEARLY

Scientific and Technical Information Center

SEARCH REQUEST FORM

Requester's Full Name: Marcela Cordero Garcia Examiner #: 80381 Date: 3/1/06

Art Unit: 1654 Phone Number: 2- _____ Serial Number: 10/822639

Location (Bldg/Room#): REM3C35 (Mailbox #): 3C18 Results Format Preferred (circle): PAPER DISK

****

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: _____

Inventors (please provide full names): _____

_____

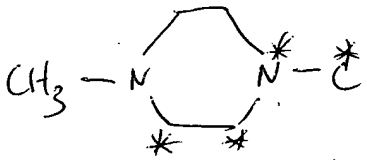
Earliest Priority Date: _____

Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequence Searches Only *Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Examiner requested in person



label at any of 4 positions

— J. DiNatale

****

STAFF USE ONLY

Searcher: _____

Searcher Phone #: _____

Searcher Location: _____

Date Searcher Picked Up: _____

Date Completed: _____

Searcher Prep & Review Time: _____

Online Time: _____

Type of Search

_____ NA Sequence (#)

_____ AA Sequence (#)

_____ Structure (#)

_____ Bibliographic

_____ Litigation

_____ Fulltext

_____ Other

Vendors and cost where applicable

_____ STN _____ Dialog

_____ Questel/Orbit _____ Lexis/Nexis

_____ Westlaw _____ WWW/Internet

____In-house sequence systems

____Commercial ____Oligomer ____Score/Length

____ Interference ____ SPDI ____ Encode/Transl

_____ Other (specify)

ACCESS DB # 176380

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Scientific and Technical Information Center

SEARCH REQUEST FORM

Requester's Full Name: MARCELA M CORDERO GARCIA Examiner #: 80381 Date: 1/11/06

Art Unit: 1654 Phone Number: 2-2939 Serial Number: 10/822,639

Location (Bldg/Room#): REM3C35 (Mailbox #): 3C18 Results Format Preferred (circle): PAPER DISK

****

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following: MG

Title of Invention: MIXTURES OF ISOBARICALLY LABELED ANALYTES AND...

Inventors (please provide full names): (SEE ATTACHD BIBDS)

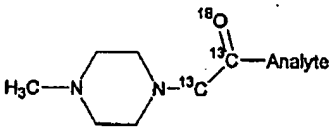
Earliest Priority Date: 1/5/04

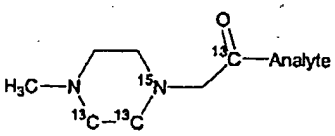
Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequence Searches Only *Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

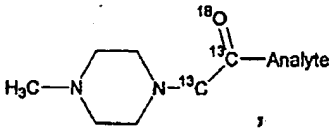
PLEASE SEARCH A MIXTURE OF THE COMPOUNDS:





, WHEREIN ANALYTE = PEPTIDE / PROTEIN

IF ONLY APPLICANT'S OWN WORK FOUND, PLEASE BROADEN SEARCH TO ENCOMPASS AT LEAST TWO OF THE FOLLOWING COMPOUNDS:



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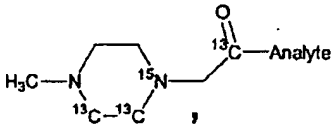

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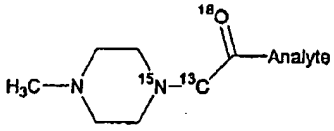
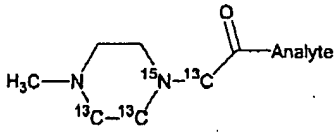


and



, WHEREIN ANALYTE = OPEN (ANY MOLECULE) OR ATOMS

THANKS, Marcela

****

STAFF USE ONLY	Type of Search	Vendors and cost where applicable
Searcher: _____	____ NA Sequence (#)	____ STN ____ Dialog
Searcher Phone #: _____	____ AA Sequence (#)	____ Questel/Orbit ____ Lexis/Nexis
Searcher Location: _____	____ Structure (#)	____ Westlaw ____ WWW/Internet
Date Searcher Picked Up: _____	____ Bibliographic	____ In-house sequence systems
Date Completed: 3/1	____ Litigation	____ Commercial ____ Oligomer ____ Score/Length
Searcher Prep & Review Time: _____	____ Fulltext	____ Interference ____ SPDI ____ Encode/Transl
Online Time: _____	____ Other	____ Other (specify)

Search history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=> d his full

     (FILE 'HOME' ENTERED AT 13:36:34 ON 01 MAR 2006)

     FILE 'REGISTRY' ENTERED AT 13:36:38 ON 01 MAR 2006
L1             STRUCTURE UPLOADED
L2          50 SEA SSS SAM L1
L3       85352 SEA SSS FUL L1
               SAVE TEMP L3 COR639STRA/A
L4             SCREEN 2039
L5           7 SEA SUB=L3 SSS SAM (L1 AND L4)
               D SCA
L6         234 SEA SUB=L3 SSS FUL (L1 AND L4)

     FILE 'CAPLUS' ENTERED AT 13:42:48 ON 01 MAR 2006
L7         127 SEA ABB=ON  PLU=ON  L6

     FILE 'STNGUIDE' ENTERED AT 13:43:18 ON 01 MAR 2006

     FILE 'REGISTRY' ENTERED AT 13:43:40 ON 01 MAR 2006
               SAVE TEMP L6 COR639ASCR/A

     FILE 'STNGUIDE' ENTERED AT 13:44:20 ON 01 MAR 2006

     FILE 'REGISTRY' ENTERED AT 13:51:13 ON 01 MAR 2006
L8             STRUCTURE UPLOADED
L9           0 SEA SUB=L3 SSS SAM L8
L10         55 SEA SUB=L3 SSS FUL L8
               SAVE TEMP L10 COR639STRB/A

     FILE 'CAPLUS' ENTERED AT 13:55:08 ON 01 MAR 2006
L11        30 SEA ABB=ON  PLU=ON  L10

     FILE 'REGISTRY' ENTERED AT 13:55:27 ON 01 MAR 2006

     FILE 'STNGUIDE' ENTERED AT 13:57:11 ON 01 MAR 2006

     FILE 'CAPLUS' ENTERED AT 14:06:04 ON 01 MAR 2006
L12     44703 SEA ABB=ON  PLU=ON  L3

     FILE 'REGISTRY' ENTERED AT 14:07:35 ON 01 MAR 2006
L*** DEL     55 S L10 AND L6
L13        179 SEA ABB=ON  PLU=ON  L6 NOT L10
L14      10857 SEA ABB=ON  PLU=ON  LABEL?
L15         14 SEA ABB=ON  PLU=ON  L14 AND L3
               D SCA
L16        256 SEA ABB=ON  PLU=ON  "CARBON-11"
L17          1 SEA ABB=ON  PLU=ON  L15 AND L16
L18        923 SEA ABB=ON  PLU=ON  "CARBON-13"
L19       3243 SEA ABB=ON  PLU=ON  "CARBON-14"
L20          6 SEA ABB=ON  PLU=ON  (L16 OR L18 OR L19) AND L3
               D SCA
L21          6 SEA ABB=ON  PLU=ON  L10 AND L20
L22        264 SEA ABB=ON  PLU=ON  NITROGEN-15
L23          0 SEA ABB=ON  PLU=ON  L22 AND L3

     FILE 'CAPLUS' ENTERED AT 14:15:33 ON 01 MAR 2006

     FILE 'HCAPLUS' ENTERED AT 14:15:47 ON 01 MAR 2006
L24     14805 SEA ABB=ON  PLU=ON  N15/OBI OR N-15/OBI OR NITROGEN-15/OBI OR
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                (NITROGEN/OBI (2A) ISOTOP?/OBI)
L25         86488 SEA ABB=ON  PLU=ON  C11/OBI OR C-11/OBI OR CARBON 11/OBI OR
                  C13/OBI OR C 13/OBI OR CARBON 13/OBI OR C14/OBI OR C 14/OBI OR
                  CARBON 14/OBI
L26         97727 SEA ABB=ON  PLU=ON  L24 OR L25
L27           112 SEA ABB=ON  PLU=ON  L26 AND L12
L28           102 SEA ABB=ON  PLU=ON  L27 NOT L11
L29            97 SEA ABB=ON  PLU=ON  L7 NOT L11
L30            90 SEA ABB=ON  PLU=ON  L28 NOT L29

     FILE 'REGISTRY' ENTERED AT 14:21:24 ON 01 MAR 2006
L31           179 SEA ABB=ON  PLU=ON  L6 NOT L10

     FILE 'HCAPLUS' ENTERED AT 14:22:59 ON 01 MAR 2006

     FILE 'STNGUIDE' ENTERED AT 14:25:55 ON 01 MAR 2006

     FILE 'HCAPLUS' ENTERED AT 14:34:04 ON 01 MAR 2006
L32         54301 SEA ABB=ON  PLU=ON  CARBON 13/OBI
L*** DEL        1 S NOTROGEN 15
L33         11153 SEA ABB=ON  PLU=ON  NITROGEN 15/OBI
L34         62382 SEA ABB=ON  PLU=ON  L32 OR L33
L35            58 SEA ABB=ON  PLU=ON  L34 AND L12
L36        428770 SEA ABB=ON  PLU=ON  LABEL?/BI
L37             3 SEA ABB=ON  PLU=ON  L35 AND L36
                  D SCA
L38             4 SEA ABB=ON  PLU=ON  L20

     FILE 'CAPLUS' ENTERED AT 14:44:58 ON 01 MAR 2006
                  E US2004-882493/APPS
L*** DEL        1 S US2004-882493/AP
                  SEL RN

     FILE 'REGISTRY' ENTERED AT 14:46:03 ON 01 MAR 2006
L*** DEL       71 S E1-E71

     FILE 'CAPLUS' ENTERED AT 14:46:16 ON 01 MAR 2006
L*** DEL   229754 S L40
                  E WO2001-012242/PN
L*** DEL        1 S WO2001-012242/PN
L*** DEL        0 S L41 AND L42
                  SEL RN L42

     FILE 'REGISTRY' ENTERED AT 14:48:30 ON 01 MAR 2006
L*** DEL       13 S E1-E13
                  D SCA

     FILE 'CAPLUS' ENTERED AT 14:49:45 ON 01 MAR 2006
                  D SCA TI L39
                  D IALL L39 1
                  SEL RN L42
                  D IALL L42
                  E WO2002-012242/PN
L*** DEL        1 S WO2002-012242/PN
                  SEL RN

     FILE 'REGISTRY' ENTERED AT 14:55:52 ON 01 MAR 2006

     FILE 'CAPLUS' ENTERED AT 14:56:02 ON 01 MAR 2006
L*** DEL          TRA L45 1- RN :     1185 TERMS
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     FILE 'REGISTRY' ENTERED AT 14:56:11 ON 01 MAR 2006
L*** DEL   1185 SEA L46
L*** DEL      3 S L40 AND L47
               D SCA

     FILE 'STNGUIDE' ENTERED AT 14:58:59 ON 01 MAR 2006

     FILE 'HCAPLUS' ENTERED AT 15:07:52 ON 01 MAR 2006

     FILE 'STNGUIDE' ENTERED AT 15:08:49 ON 01 MAR 2006

     FILE 'HCAPLUS' ENTERED AT 15:09:22 ON 01 MAR 2006
L39        12370 SEA ABB=ON  PLU=ON  C 13/BI
L40         6125 SEA ABB=ON  PLU=ON  N 15/BI
L41        18437 SEA ABB=ON  PLU=ON  (L39 OR L40)
L42           49 SEA ABB=ON  PLU=ON  L41 AND L12
L43        44703 SEA ABB=ON  PLU=ON  L3
L44           49 SEA ABB=ON  PLU=ON  L41 AND L43
L45            0 SEA ABB=ON  PLU=ON  L41 AND L43 AND L36
L46        55408 SEA ABB=ON  PLU=ON  CARBON 13/BI
L47        11292 SEA ABB=ON  PLU=ON  NITROGEN 15/BI
L48        80814 SEA ABB=ON  PLU=ON  L46 OR L47 OR L39 OR L40
L49          109 SEA ABB=ON  PLU=ON  L48 AND L43
L50           30 SEA ABB=ON  PLU=ON  L10
L51            4 SEA ABB=ON  PLU=ON  L20
L52          108 SEA ABB=ON  PLU=ON  L49 NOT ((L50 OR L51))
L53       647038 SEA ABB=ON  PLU=ON  ?ENRICH?/BI OR ?LABEL?/BI
L54            5 SEA ABB=ON  PLU=ON  L48 AND L43 AND L53
               D SCA
L55         4422 SEA ABB=ON  PLU=ON  NATURAL ABUND?/BI
L56            3 SEA ABB=ON  PLU=ON  L48 AND L43 AND L55
               D SCA
L57        20665 SEA ABB=ON  PLU=ON  (C 13/OBI OR CARBON 13/OBI OR N 15/OBI OR
               NITROGEN 15/OBI) (W) (NUCLEAR MAGNET?/OBI OR NMR/OBI)
L58           81 SEA ABB=ON  PLU=ON  L49 NOT L57

     FILE 'STNGUIDE' ENTERED AT 15:19:00 ON 01 MAR 2006

     FILE 'HCAPLUS' ENTERED AT 15:19:43 ON 01 MAR 2006
               E US2004-822639/APPS
L59            6 SEA ABB=ON  PLU=ON  (US2004-822639/AP OR US2004-822639/PRN)
               D SCA
L60       321506 SEA ABB=ON  PLU=ON  ISOTOP?/BI
L61            5 SEA ABB=ON  PLU=ON  L49 AND L60
L62        17234 SEA ABB=ON  PLU=ON  ISOBAR?/BI
L63            0 SEA ABB=ON  PLU=ON  L49 AND L62
L64       392306 SEA ABB=ON  PLU=ON  FRAGMENT?/BI
L65            5 SEA ABB=ON  PLU=ON  L64 AND L49
               D SCA
L66            9 SEA ABB=ON  PLU=ON  L37 OR L61 OR L63 OR L65
L67           30 SEA ABB=ON  PLU=ON  (L50 OR L51)
L68            1 SEA ABB=ON  PLU=ON  L66 AND L67
L69        14811 SEA ABB=ON  PLU=ON  L3 (L) PREP/RL
L70           32 SEA ABB=ON  PLU=ON  L69 AND L48
L71           30 SEA ABB=ON  PLU=ON  L70 NOT ((L66 OR L67))
               D COST

     FILE 'STNGUIDE' ENTERED AT 15:31:24 ON 01 MAR 2006
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     FILE 'HCAPLUS' ENTERED AT 15:45:44 ON 01 MAR 2006
L72          503 SEA ABB=ON  PLU=ON  LABEL?/BI (L) PIPERAZ?/BI
L73            1 SEA ABB=ON  PLU=ON  L72 AND L49
L74          936 SEA ABB=ON  PLU=ON  ?LABEL?/BI (L) ?PIPERAZ?/BI
L75            1 SEA ABB=ON  PLU=ON  L74 AND L49
L76          450 SEA ABB=ON  PLU=ON  ?LABEL?/BI (S) ?PIPERAZ?/BI
L77            1 SEA ABB=ON  PLU=ON  L76 AND L49
L78           92 SEA ABB=ON  PLU=ON  ?ENRICH?/BI (L) ?PIPERAZ?/BI
L79            0 SEA ABB=ON  PLU=ON  L78 AND L49
L80           92 SEA ABB=ON  PLU=ON  ?ENRICH?/BI (P) ?PIPERAZ?/BI
L81          110 SEA ABB=ON  PLU=ON  PAPPIN D?/AU
L82           45 SEA ABB=ON  PLU=ON  PURKAYASTHA, S?/AU
L83          168 SEA ABB=ON  PLU=ON  COULL, J?/AU
L84           14 SEA ABB=ON  PLU=ON  (L81 AND (L82 OR L83)) OR (L82 AND L83)

     FILE 'REGISTRY' ENTERED AT 15:51:11 ON 01 MAR 2006
L85              ANALYZE PLU=ON  L10 1- LC :       6 TERMS
                 D

     FILE 'USPATFULL' ENTERED AT 15:53:12 ON 01 MAR 2006
L86           11 SEA ABB=ON  PLU=ON  L10
L87            8 SEA ABB=ON  PLU=ON  (L81 AND (L82 OR L83)) OR (L82 AND L83)

     FILE 'STNGUIDE' ENTERED AT 15:55:15 ON 01 MAR 2006

     FILE 'HCAPLUS' ENTERED AT 15:55:26 ON 01 MAR 2006
L88            6 SEA ABB=ON  PLU=ON  L84 AND ((L50 OR L51) OR L37 OR L61 OR L63
                 OR L65 OR L54 OR L75 OR L79)
L89            6 SEA ABB=ON  PLU=ON  L86 AND L87

     FILE 'STNGUIDE' ENTERED AT 15:56:58 ON 01 MAR 2006

     FILE 'REGISTRY' ENTERED AT 15:57:15 ON 01 MAR 2006
               D STAT QUE L10
               D STAT QUE L20
               D STAT QUE L23

     FILE 'STNGUIDE' ENTERED AT 15:58:00 ON 01 MAR 2006

     FILE 'HCAPLUS' ENTERED AT 15:59:10 ON 01 MAR 2006
               D QUE NOS L84
               D QUE NOS L88
L90           14 SEA ABB=ON  PLU=ON  L84 OR L88

     FILE 'USPATFULL' ENTERED AT 15:59:15 ON 01 MAR 2006
               D QUE NOS L87
               D QUE NOS L89
L91            8 SEA ABB=ON  PLU=ON  L87 OR L89

     FILE 'STNGUIDE' ENTERED AT 15:59:26 ON 01 MAR 2006

     FILE 'HCAPLUS, USPATFULL' ENTERED AT 15:59:49 ON 01 MAR 2006
L92           16 DUP REM L90 L91 (6 DUPLICATES REMOVED)
                    ANSWERS '1-14' FROM FILE HCAPLUS
                    ANSWERS '15-16' FROM FILE USPATFULL
                 D IBIB ABS HITIND HITSTR L92 1-14
                 D IBIB ABS KWIC HITSTR L92 15-16

     FILE 'STNGUIDE' ENTERED AT 16:01:20 ON 01 MAR 2006
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     FILE 'HCAPLUS' ENTERED AT 16:03:38 ON 01 MAR 2006
                D QUE NOS L50
                D QUE NOS L51
                D QUE NOS L37
                D QUE NOS L61
                D QUE NOS L63
                D QUE NOS L65
                D QUE NOS L54
                D QUE NOS L75
                D QUE NOS L79
L93           34 SEA ABB=ON  PLU=ON  (L50 OR L51 OR L37 OR L61 OR L63 OR L65 OR
                L54 OR L75 OR L79) NOT L90

     FILE 'USPATFULL' ENTERED AT 16:03:46 ON 01 MAR 2006
                D QUE NOS L86
L94            5 SEA ABB=ON  PLU=ON  L86 NOT L91

     FILE 'STNGUIDE' ENTERED AT 16:04:06 ON 01 MAR 2006

     FILE 'HCAPLUS, USPATFULL' ENTERED AT 16:04:46 ON 01 MAR 2006
L95           37 DUP REM L93 L94 (2 DUPLICATES REMOVED)
                     ANSWERS '1-34' FROM FILE HCAPLUS
                     ANSWERS '35-37' FROM FILE USPATFULL
                D IBIB ABS HITIND HITSTR L95 1-34
                D IBIB ABS KWIC HITSTR L95 35-37


     FILE HOME

     FILE REGISTRY
     Property values tagged with IC are from the ZIC/VINITI data file
     provided by InfoChem.

     STRUCTURE FILE UPDATES:   28 FEB 2006  HIGHEST RN 875516-18-0
     DICTIONARY FILE UPDATES:  28 FEB 2006  HIGHEST RN 875516-18-0

     New CAS Information Use Policies, enter HELP USAGETERMS for details.

     TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

       Please note that search-term pricing does apply when
       conducting SmartSELECT searches.

     ************************************************************
     *                                                          *
     * The CA roles and document type information have been removed from *
     * the IDE default display format and the ED field has been added,   *
     * effective March 20, 2005.  A new display format, IDERL, is now    *
     * available and contains the CA role and document type information. *
     *                                                          *
     ************************************************************

     Structure search iteration limits have been increased.  See HELP SLIMITS
     for details.

     REGISTRY includes numerically searchable data for experimental and
     predicted properties as well as tags indicating availability of
     experimental property data in the original document.  For information
     on property searching in REGISTRY, refer to:
```

http://www.cas.org/ONLINE/UG/regprops.html

FILE CAPLUS

FILE COVERS 1907 - 1 Mar 2006 VOL 144 ISS 10
FILE LAST UPDATED: 28 Feb 2006 (20060228/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

FILE STNGUIDE
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Feb 24, 2006 (20060224/UP).

FILE HCAPLUS

FILE COVERS 1907 - 1 Mar 2006 VOL 144 ISS 10
FILE LAST UPDATED: 28 Feb 2006 (20060228/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE USPATFULL
FILE COVERS 1971 TO PATENT PUBLICATION DATE: 28 Feb 2006 (20060228/PD)
FILE LAST UPDATED: 28 Feb 2006 (20060228/ED)
HIGHEST GRANTED PATENT NUMBER: US7007305
HIGHEST APPLICATION PUBLICATION NUMBER: US2006041984
CA INDEXING IS CURRENT THROUGH 28 Feb 2006 (20060228/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 28 Feb 2006 (20060228/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Dec 2005
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Dec 2005

=>

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=> file registry
FILE 'REGISTRY' ENTERED AT 15:57:15 ON 01 MAR 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2006 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   28 FEB 2006  HIGHEST RN 875516-18-0
DICTIONARY FILE UPDATES:  28 FEB 2006  HIGHEST RN 875516-18-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

*************************************************************************
*                                                                       *
* The CA roles and document type information have been removed from     *
* the IDE default display format and the ED field has been added,       *
* effective March 20, 2005.  A new display format, IDERL, is now        *
* available and contains the CA role and document type information.     *
*                                                                       *
*************************************************************************

Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> d stat que L10
L1                STR
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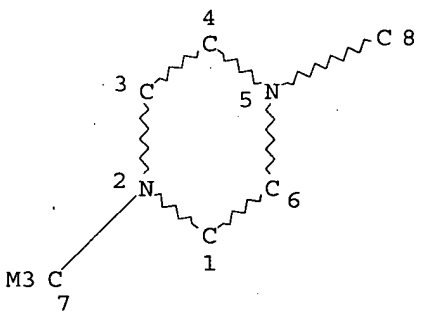


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NODE ATTRIBUTES:
HCOUNT   IS M3     AT   7
NSPEC    IS R      AT   1
NSPEC    IS R      AT   2
NSPEC    IS R      AT   3
NSPEC    IS R      AT   4
NSPEC    IS R      AT   5
```

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NSPEC   IS R      AT   6
NSPEC   IS C      AT   7
NSPEC   IS RC     AT   8
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT   7  8
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   8

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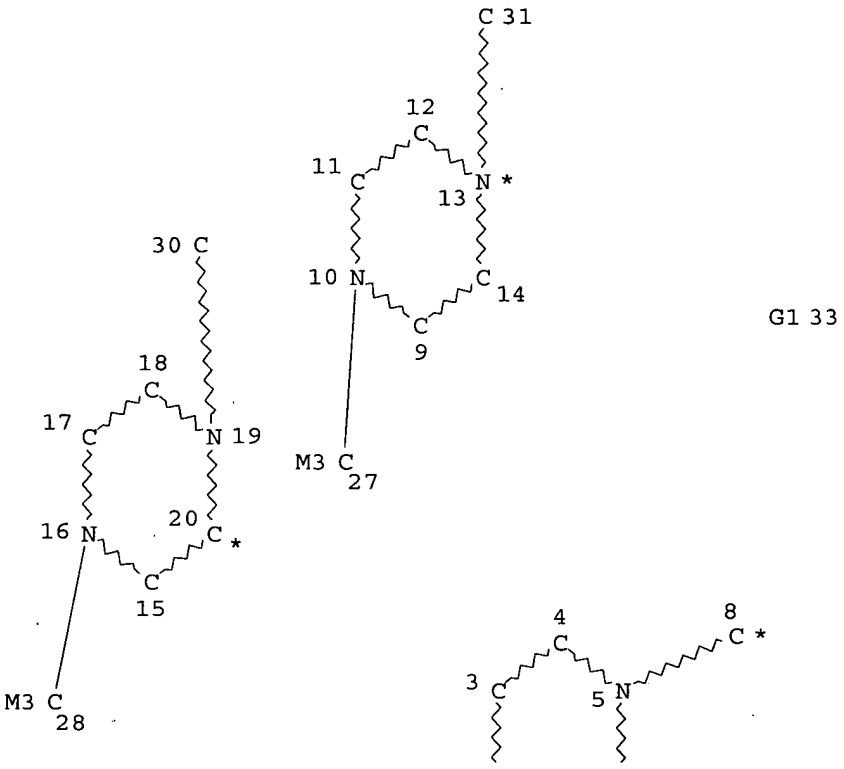
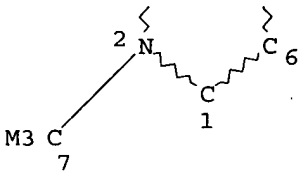
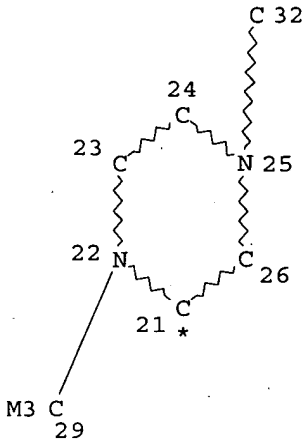


Page 1-A





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HCOUNT	IS M3	AT	27
HCOUNT	IS M3	AT	28
HCOUNT	IS M3	AT	29
MASS	IS *	AT	8
MASS	IS *	AT	13
MASS	IS *	AT	20
MASS	IS *	AT	21
NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS C	AT	7
NSPEC	IS RC	AT	8
NSPEC	IS R	AT	9
NSPEC	IS R	AT	10
NSPEC	IS R	AT	11
NSPEC	IS R	AT	12
NSPEC	IS R	AT	13
NSPEC	IS R	AT	14
NSPEC	IS R	AT	15
NSPEC	IS R	AT	16
NSPEC	IS R	AT	17
NSPEC	IS R	AT	18
NSPEC	IS R	AT	19

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NSPEC   IS R      AT  20
NSPEC   IS R      AT  21
NSPEC   IS R      AT  22
NSPEC   IS R      AT  23
NSPEC   IS R      AT  24
NSPEC   IS R      AT  25
NSPEC   IS R      AT  26
NSPEC   IS C      AT  27
NSPEC   IS C      AT  28
NSPEC   IS C      AT  29
NSPEC   IS RC     AT  30
NSPEC   IS RC     AT  31
NSPEC   IS RC     AT  32
NSPEC   IS C      AT  33
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT   7  8 27 28 29 30 31 32
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  33

STEREO ATTRIBUTES: NONE
L10          55 SEA FILE=REGISTRY SUB=L3 SSS FUL L8

100.0% PROCESSED   85352 ITERATIONS                          55 ANSWERS
SEARCH TIME: 00.00.01


=> d stat que L20
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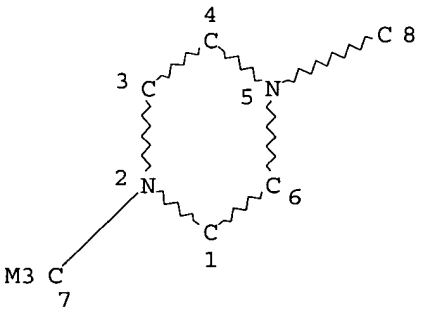


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NSPEC   IS R      AT   1
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NSPEC   IS C      AT   7
NSPEC   IS RC     AT   8
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT   7  8
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   8

STEREO ATTRIBUTES: NONE
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L16          256 SEA FILE=REGISTRY ABB=ON  PLU=ON  "CARBON-11"
L18          923 SEA FILE=REGISTRY ABB=ON  PLU=ON  "CARBON-13"
L19         3243 SEA FILE=REGISTRY ABB=ON  PLU=ON  "CARBON-14"
L20            6 SEA FILE=REGISTRY ABB=ON  PLU=ON  (L16 OR L18 OR L19) AND L3


=> d stat que L23
L1                STR
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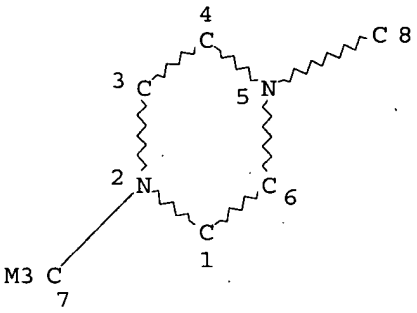


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HCOUNT  IS M3     AT   7
NSPEC   IS R      AT   1
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DEFAULT MLEVEL IS ATOM
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DEFAULT ECLEVEL IS LIMITED

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RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   8

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L22          264 SEA FILE=REGISTRY ABB=ON  PLU=ON  NITROGEN-15
L23            0 SEA FILE=REGISTRY ABB=ON  PLU=ON  L22 AND L3


=> => file hcaplus
FILE 'HCAPLUS' ENTERED AT 15:59:10 ON 01 MAR 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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```

AUTHOR SEARCH

FILE COVERS 1907 - 1 Mar 2006 VOL 144 ISS 10
FILE LAST UPDATED: 28 Feb 2006 (20060228/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate
substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d que nos L84

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L81          110 SEA FILE=HCAPLUS ABB=ON  PLU=ON  PAPPIN D?/AU
L82           45 SEA FILE=HCAPLUS ABB=ON  PLU=ON  PURKAYASTHA, S?/AU '
L83          168 SEA FILE=HCAPLUS ABB=ON  PLU=ON  COULL, J?/AU
L84           14 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L81 AND (L82 OR L83)) OR
                    (L82 AND L83)
```

=> d que nos L88

```
L1               STR
L3         85352 SEA FILE=REGISTRY SSS FUL L1
L8               STR
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L12        44703 SEA FILE=CAPLUS ABB=ON  PLU=ON  L3
L16          256 SEA FILE=REGISTRY ABB=ON  PLU=ON  "CARBON-11"
L18          923 SEA FILE=REGISTRY ABB=ON  PLU=ON  "CARBON-13"
L19         3243 SEA FILE=REGISTRY ABB=ON  PLU=ON  "CARBON-14"
L20            6 SEA FILE=REGISTRY ABB=ON  PLU=ON  (L16 OR L18 OR L19) AND L3
L32        54301 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CARBON 13/OBI
L33        11153 SEA FILE=HCAPLUS ABB=ON  PLU=ON  NITROGEN 15/OBI
L34        62382 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L32 OR L33
L35           58 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L34 AND L12
L36       428770 SEA FILE=HCAPLUS ABB=ON  PLU=ON  LABEL?/BI
L37            3 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L35 AND L36
L39        12370 SEA FILE=HCAPLUS ABB=ON  PLU=ON  C 13/BI
L40         6125 SEA FILE=HCAPLUS ABB=ON  PLU=ON  N 15/BI
L43        44703 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L3
L46        55408 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CARBON 13/BI
L47        11292 SEA FILE=HCAPLUS ABB=ON  PLU=ON  NITROGEN 15/BI
L48        80814 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L46 OR L47 OR L39 OR L40
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L50           30 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L10
L51            4 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20
L53       647038 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ?ENRICH?/BI OR ?LABEL?/BI
L54            5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L48 AND L43 AND L53
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L62        17234 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ISOBAR?/BI
L63            0 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L49 AND L62
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L75           1 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L74 AND L49
L78          92 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ?ENRICH?/BI (L) ?PIPERAZ?/BI
L79           0 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L78 AND L49
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L82          45 SEA FILE=HCAPLUS ABB=ON  PLU=ON  PURKAYASTHA, S?/AU
L83         168 SEA FILE=HCAPLUS ABB=ON  PLU=ON  COULL, J?/AU
L84          14 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L81 AND (L82 OR L83)) OR
                (L82 AND L83)
L88           6 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L84 AND ((L50 OR L51) OR L37
                OR L61 OR L63 OR L65 OR L54 OR L75 OR L79)


=> s L84 or L88

L90          14 L84 OR L88

=> file uspatfull

FILE 'USPATFULL' ENTERED AT 15:59:15 ON 01 MAR 2006
CA INDEXING COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 28 Feb 2006 (20060228/PD)
FILE LAST UPDATED: 28 Feb 2006 (20060228/ED)
HIGHEST GRANTED PATENT NUMBER: US7007305
HIGHEST APPLICATION PUBLICATION NUMBER: US2006041984
CA INDEXING IS CURRENT THROUGH 28 Feb 2006 (20060228/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 28 Feb 2006 (20060228/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Dec 2005
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Dec 2005


=> d que nos L87

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L82          45 SEA FILE=HCAPLUS ABB=ON  PLU=ON  PURKAYASTHA, S?/AU
L83         168 SEA FILE=HCAPLUS ABB=ON  PLU=ON  COULL, J?/AU
L87           8 SEA FILE=USPATFULL ABB=ON  PLU=ON  (L81 AND (L82 OR L83)) OR
                (L82 AND L83)


=> d que nos L89

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L8              STR
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L82            45 SEA FILE=HCAPLUS ABB=ON  PLU=ON  PURKAYASTHA, S?/AU
L83           168 SEA FILE=HCAPLUS ABB=ON  PLU=ON  COULL, J?/AU
L86            11 SEA FILE=USPATFULL ABB=ON  PLU=ON  L10
L87             8 SEA FILE=USPATFULL ABB=ON  PLU=ON  (L81 AND (L82 OR L83)) OR
                (L82 AND L83)
L89             6 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L86 AND L87


=> s L87 or L89

L91             8 L87 OR L89

=> => dup rem L90 L91
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FILE 'HCAPLUS' ENTERED AT 15:59:49 ON 01 MAR 2006
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FILE 'USPATFULL' ENTERED AT 15:59:49 ON 01 MAR 2006
CA INDEXING COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)
PROCESSING COMPLETED FOR L90
PROCESSING COMPLETED FOR L91
L92           16 DUP REM L90 L91 (6 DUPLICATES REMOVED)
                 ANSWERS '1-14' FROM FILE HCAPLUS
                 ANSWERS '15-16' FROM FILE USPATFULL

=> d ibib abs hitind hitstr L92 1-14; d ibib abs kwic hitstr L92 15-16

L92  ANSWER 1 OF 16  HCAPLUS  COPYRIGHT 2006 ACS on STN DUPLICATE 1
ACCESSION NUMBER:         2005:588426  HCAPLUS
DOCUMENT NUMBER:          143:115568
TITLE:                    Preparation of isotopically enriched N-substituted
                          piperazine-1-acetic acids
INVENTOR(S):              Dey, Subhakar; Pappin, Darryl J. c.;
                          Purkayastha, Subhasish; Pillai, Sasi;
                          Coull, James M.
PATENT ASSIGNEE(S):       Applera Corp., USA
SOURCE:                   U.S. Pat. Appl. Publ., 29 pp.
                          CODEN: USXXCO
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   6
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
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     US 2005148774         A1    20050707    US 2004-751387          20040105
     WO 2005068446         A1    20050728    WO 2005-US223           20050105
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
             RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
             MR, NE, SN, TD, TG
PRIORITY APPLN. INFO.:                   US 2004-751353      A  20040105
                                         US 2004-751354      A  20040105
                                         US 2004-751387      A  20040105
                                         US 2004-751388      A  20040105
                                         US 2004-822639      A  20040412
                                         US 2004-852730      A  20040524
OTHER SOURCE(S):          MARPAT 143:115568
GI
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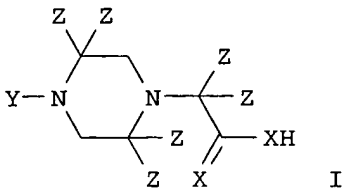


I

AB Isotopically enriched N-substituted piperazine-1-acetic acids (I) or salts thereof, comprising one or more heavy atom isotopes [X = O, S; Y = straight chain or branched C1-6 alkyl or C1-6 alkyl ether group wherein the carbon atoms of the alkyl group or alkyl ether group each independently comprise linked hydrogen, deuterium or F atoms; Z = independently H, deuterium, F, Cl, Br, iodine, an amino acid side chain, a straight chain or branched C1-6 alkyl group that may optionally contain a substituted or unsubstituted aryl group (wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H, deuterium or F atoms), a straight chain or branched C1-6 alkyl ether group that may optionally contain a substituted or unsubstituted aryl group wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H, deuterium or F atoms, or a straight chain or branched C1-6 alkoxy group that may optionally contain a substituted or unsubstituted aryl group (wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H, deuterium or F atoms)] are prepared N-substituted piperazines can be used as intermediates in the synthesis of N-substituted piperazine acetic acids which in turn can be used as intermediates in the synthesis of active esters of N-substituted piperazine acetic acid. The active esters of N-substituted piperazine acetic acid can be used as labeling reagents to prepare a set of isobaric labeling reagents. The set of isobaric labeling reagents can be used to label analytes such as peptides, proteins, amino acids, oligonucleotides, DNA, RNA, lipids, carbohydrates, steroids, small mols. and the like. Thus, to a stirring solution of 1.18 g (11.83 mmol) N-methylpiperazine in 15 mL toluene at room temperature was added 1 g (5.91 mmol) of Et bromoacetate-1,2-13C dropwise, over a period of 15 min. The reaction mixture was then heated in an oil bath at 90° for 4 h, cooled to room temperature, filtered to remove the off-white solid to give, after workup on the combined filtrate and washings, 1.10 g (quant.) of 4-methylpiperazine-1-acetic acid Et ester-1,2-13C (II) as an off-white oil. II (1.1 g) was refluxed in water for 24 h to give 780 mg 4-methylpiperazine-1-acetic acid-1,2-13C.

IC ICM C07D241-04

INCL 544399000

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 6, 80

IT **856188-20-0P**
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)

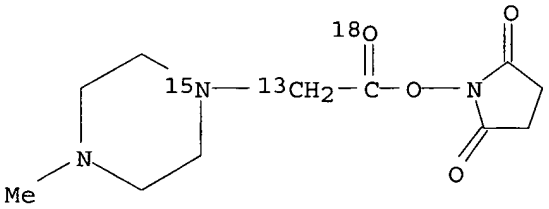
IT 79-08-3DP, Bromoacetic acid, trityl chloride resin-bound 5672-86-6P, Trifluoroacetic acid pentachlorophenyl ester 5672-89-9P, Trifluoroacetic acid succinimidyl ester 54699-92-2P, 4-Methylpiperazine-1-acetic acid 145142-92-3P 145142-94-5P **856187-64-9P** **856187-68-3P** **856187-72-9P** 856187-80-9P 856187-83-2P **856188-16-4P** 856188-80-2P 856188-88-0P, Trifluoroacetic acid 2-oxopyrrolidin-1-yl

ester 857027-04-4P 857027-05-5P 857027-07-7P 857502-95-5P
857502-96-6P 857502-97-7P 857502-98-8P
857502-99-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)

IT **856187-76-3P** 856187-87-6P **856187-92-3P** 856188-02-8P,
4-Methylpiperazine-1-acetic acid 1,1,1,3,3,3-hexafluoropropan-2-yl ester
856188-06-2P 856188-23-3P 856188-27-7P 856188-32-4P 856188-37-9P
856188-38-0P 856188-43-7P 856188-44-8P 856188-49-3P 856188-50-6P
856188-62-0P **856290-53-4P 856290-55-6P** 857027-09-9P
857027-10-2P **857027-11-3P 857027-12-4P** 857503-00-5P
857503-01-6P 857503-02-7P 857503-03-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)

IT **856188-20-0P**
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)

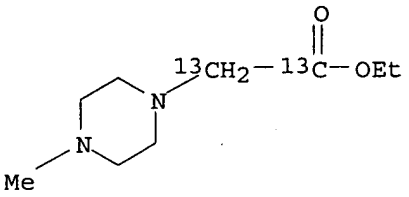
RN 856188-20-0 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl-1-15N)acetyl-2-13C-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

IT **856187-64-9P 856187-68-3P 856187-72-9P**
856188-16-4P 857502-96-6P 857502-97-7P
857502-98-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)

RN 856187-64-9 HCAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2 acid, 4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



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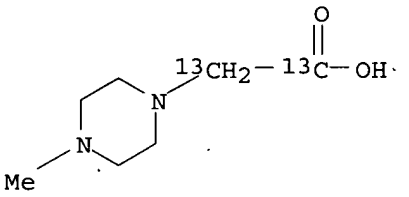

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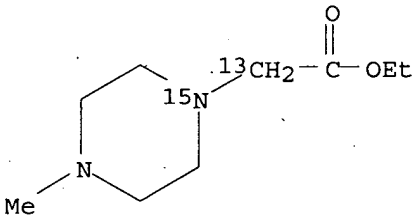

RN 856188-16-4 HCAPLUS
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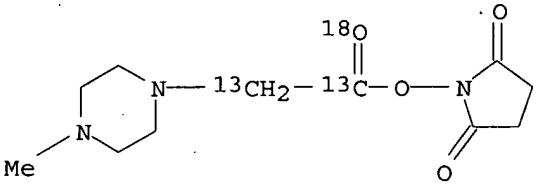
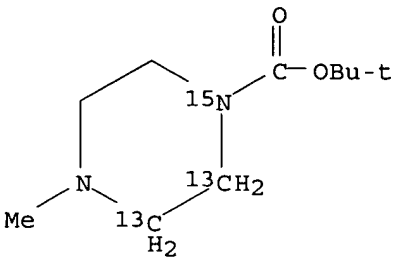
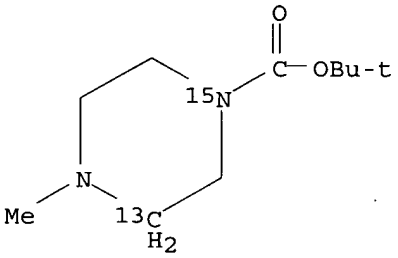


● 2 HCl

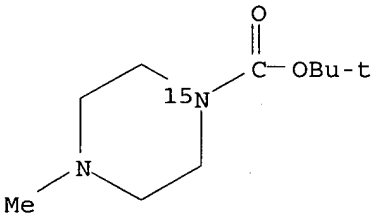
RN 857502-96-6 HCAPLUS
CN 1-Piperazine-2,3-13C2-1-15N-carboxylic acid, 4-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



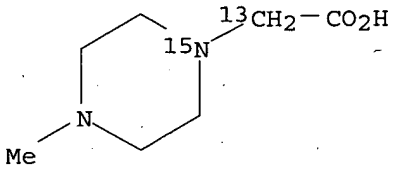
RN 857502-97-7 HCAPLUS
CN 1-Piperazine-3-13C-1-15N-carboxylic acid, 4-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



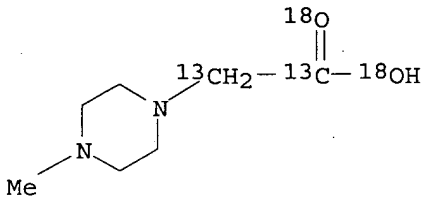
RN 857502-98-8 HCAPLUS
CN 1-Piperazine-1-15N-carboxylic acid, 4-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



IT **856187-76-3P 856187-92-3P 856290-53-4P**
856290-55-6P 857027-11-3P 857027-12-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)
RN 856187-76-3 HCAPLUS
CN 1-Piperazine-1-15N-acetic-α-13C acid, 4-methyl- (9CI) (CA INDEX NAME)

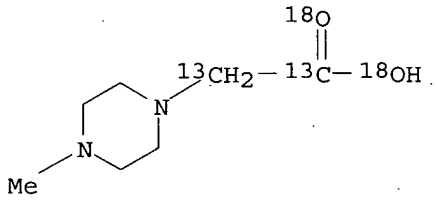


RN 856187-92-3 HCAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2-18O2 acid, 4-methyl-, dihydrochloride (9CI) (CA INDEX NAME)

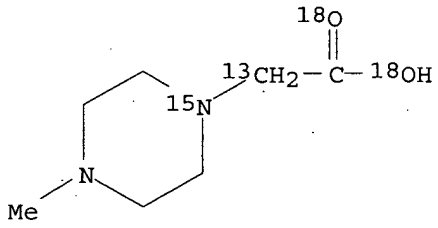


●2 HCl

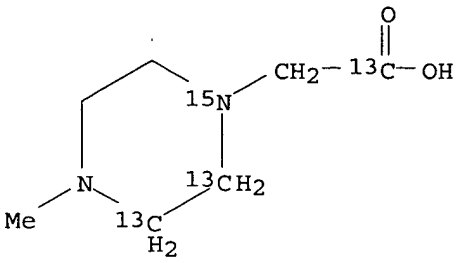
RN 856290-53-4 HCAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2-18O2 acid, 4-methyl- (9CI) (CA INDEX NAME)



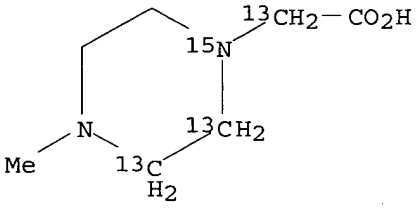
RN 856290-55-6 HCAPLUS
CN 1-Piperazineacetic-α-13C-1-15N-18O2 acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 857027-11-3 HCAPLUS
CN 1-Piperazine-2,3-13C2-1-15N-acetic-carboxy-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 857027-12-4 HCAPLUS
CN 1-Piperazine-2,3-13C2-1-15N-acetic-α-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



L92 ANSWER 2 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 2005:592130 HCAPLUS
DOCUMENT NUMBER: 143:115574
TITLE: Preparation of isotopically enriched N-substituted piperazines
INVENTOR(S): **Pappin, Darryl J. C.**; Pillai, Sasi; **Coull, James M.**
PATENT ASSIGNEE(S): Applera Corp., USA
SOURCE: U.S. Pat. Appl. Publ., 29 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005148773	A1	20050707	US 2004-751388	20040105
WO 2005068446	A1	20050728	WO 2005-US223	20050105

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

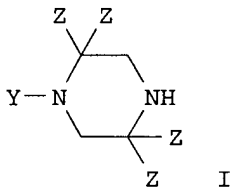
PRIORITY APPLN. INFO.:

US 2004-751353	A	20040105
US 2004-751354	A	20040105
US 2004-751387	A	20040105

US 2004-751388 A 20040105
US 2004-822639 A 20040412
US 2004-852730 A 20040524

OTHER SOURCE(S): MARPAT 143:115574

GI



I

AB Isotopically enriched N-substituted piperazines (I) or salts thereof, comprising one or more heavy atom isotopes (Y = straight chain or branched C1-6 alkyl or C1-6 alkyl ether group wherein the carbon atoms of the alkyl group or alkyl ether group each independently comprise linked hydrogen, deuterium or fluorine atoms; Z = independently H, F, Cl, Br, iodine, an amino acid side chain, a straight chain or branched C1-6 alkyl group that may optionally contain a substituted or unsubstituted aryl group wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H or F atoms, a straight chain or branched C1-6 alkyl ether group that may optionally contain a substituted or unsubstituted aryl group (wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked hydrogen or fluorine atoms), or a straight chain or branched C1-6 alkoxy group that may optionally contain a substituted or unsubstituted aryl group; wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked hydrogen or fluorine atoms; wherein the N-methylpiperazine is isotopically enriched with either of 13C and/or 15N) are prepared N-substituted piperazines can be used as intermediates in the synthesis of N-substituted piperazine acetic acids which in turn can be used as intermediates in the synthesis of active esters of N-substituted piperazine acetic acid. The active esters of N-substituted piperazine acetic acid can be used as labeling reagents to prepare a set of isobaric labeling reagents. The set of isobaric labeling reagents can be used to label analytes such as peptides, proteins, amino acids, oligonucleotides, DNA, RNA, lipids, carbohydrates, steroids, small mols. and the like (no data). Thus, to a stirring solution of 1.18 g (11.83 mmol) N-methylpiperazine in 15 mL toluene at room temperature was added 1 g (5.91 mmol) of Et bromoacetate-1,2-13C dropwise, over a period of 15 min. The reaction mixture was then heated in an oil bath at 90° for 4 h, cooled to room temperature, filtered to remove the off-white solid to give, after workup on the combined filtrate and washings, 1.10 g (quant.) of 4-methylpiperazine-1-acetic acid Et ester-1,2-13C (II) as an off-white oil. II (1.1 g) was refluxed in water for 24 h to give 780 mg 4-methylpiperazine-1-acetic acid-1,2-13C.

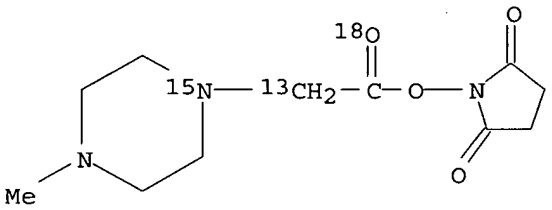
IC ICM C07D241-04
INCL 544358000
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 6, 80
IT **856188-20-0P**
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(preparation of isotopically enriched N-substituted piperazines as isobaric labeling reagents)
IT 5672-86-6P, Trifluoroacetic acid pentachlorophenyl ester 5672-89-9P,

Trifluoroacetic acid succinimidyl ester 54699-92-2P,
4-Methylpiperazine-1-acetic acid 106665-75-2P 145142-98-9P
145143-00-6P 856187-57-0P **856187-64-9P 856187-68-3P**
856187-72-9P 856187-80-9P 856187-83-2P **856187-92-3P**
856188-16-4P 856188-23-3P 856188-27-7P 856188-32-4P
856188-37-9P 856188-43-7P 856188-49-3P 856188-80-2P 856188-88-0P,
Trifluoroacetic acid 2-oxopyrrolidin-1-yl ester 856290-54-5P
857027-04-4P 857027-05-5P **857502-96-6P 857502-97-7P**
857502-98-8P 857502-99-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isotopically enriched N-substituted piperazines as isobaric labeling reagents)

IT **856187-76-3P** 856187-87-6P 856188-02-8P, 4-Methylpiperazine-1-acetic acid 1,1,1,3,3,3-hexafluoropropan-2-yl ester 856188-06-2P
856188-38-0P 856188-44-8P 856188-50-6P 856188-62-0P 857027-09-9P
857027-10-2P 857503-00-5P 857503-01-6P 857503-02-7P 857503-03-8P
857503-04-9P 857503-05-0P 857503-06-1P 857503-07-2P 857503-08-3P
857503-09-4P 857503-10-7P 857503-11-8P 857503-12-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of isotopically enriched N-substituted piperazines as isobaric labeling reagents)

IT **856188-20-0P**
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(preparation of isotopically enriched N-substituted piperazines as isobaric labeling reagents)

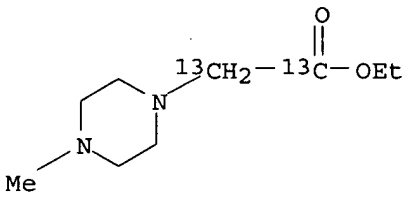
RN 856188-20-0 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl-1-15N)acetyl-2-13C-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)



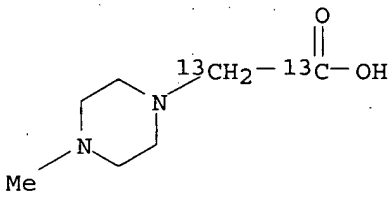
●2 HCl

IT **856187-64-9P 856187-68-3P 856187-72-9P**
856187-92-3P 856188-16-4P 857502-96-6P
857502-97-7P 857502-98-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isotopically enriched N-substituted piperazines as isobaric labeling reagents)

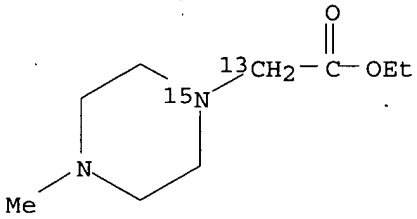
RN 856187-64-9 HCAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2 acid, 4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



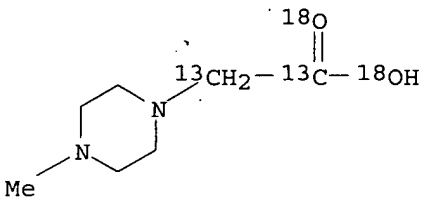
RN 856187-68-3 HCAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2 acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 856187-72-9 HCAPLUS
CN 1-Piperazine-1-15N-acetic-α-13C acid, 4-methyl-, ethyl ester (9CI) (CA INDEX NAME)

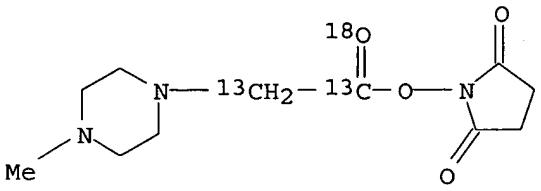


RN 856187-92-3 HCAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2-18O2 acid, 4-methyl-, dihydrochloride (9CI) (CA INDEX NAME)



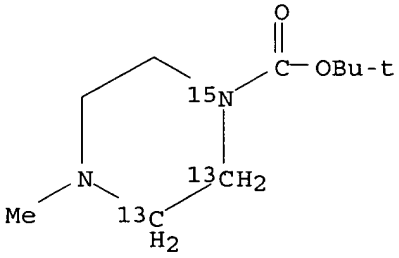
●2 HCl

RN 856188-16-4 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-13C2-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)

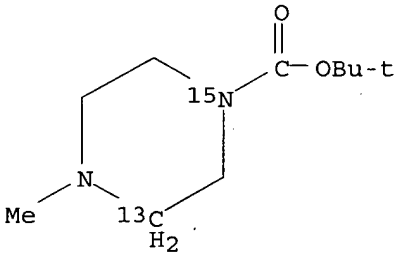


● 2 HCl

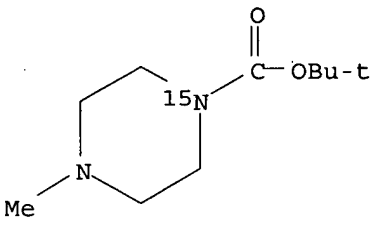
RN 857502-96-6 HCAPLUS
CN 1-Piperazine-2,3-13C2-1-15N-carboxylic acid, 4-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



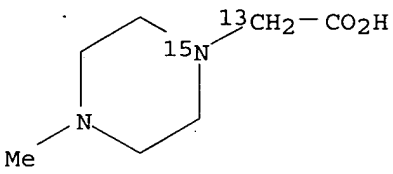
RN 857502-97-7 HCAPLUS
CN 1-Piperazine-3-13C-1-15N-carboxylic acid, 4-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 857502-98-8 HCAPLUS
CN 1-Piperazine-1-15N-carboxylic acid, 4-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



IT **856187-76-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of isotopically enriched N-substituted piperazines as isobaric labeling reagents)
RN 856187-76-3 HCAPLUS
CN 1-Piperazine-1-15N-acetic-α-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



L92 ANSWER 3 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 2005:592129 HCAPLUS
DOCUMENT NUMBER: 143:97398
TITLE: Preparation of active esters of N-substituted piperazine acetic acids, including isotopically enriched versions
INVENTOR(S): Dey, Subhakar; **Pappin, Darryl J. C.**; **Purkayastha, Subhasish**; Pillai, Sasi; **Coull, James M.**
PATENT ASSIGNEE(S): Applera Corp., USA
SOURCE: U.S. Pat. Appl. Publ., 33 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005148771	A1	20050707	US 2004-751354	20040105
WO 2005068446	A1	20050728	WO 2005-US223	20050105

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,

MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

US 2004-751353	A	20040105
US 2004-751354	A	20040105
US 2004-751387	A	20040105
US 2004-751388	A	20040105
US 2004-822639	A	20040412
US 2004-852730	A	20040524

OTHER SOURCE(S): MARPAT 143:97398

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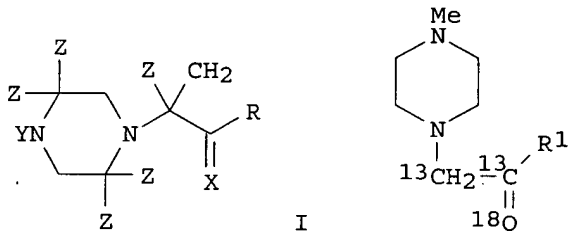


I II

AB In some embodiments, this invention pertains to active esters of N-substituted piperazine acetic acid I (R = leaving group; X = O, S; Y = C1-C6 alkyl, C1-C6 alkyl ether; Z = H, 2H, F, Cl, Br, iodide, amino acid side chain, C1-C6 alkyl, C1-C6 alkyl ether), including isotopically enriched versions thereof. In some embodiments, this invention pertains to methods for the preparation of active esters of N-substituted piperazine acetic acid, including isotopically enriched versions thereof. For example, the isotopically labeled N-methylpiperazine II (R1 = 18OH) reacted with the trifluoroacetic acid ester of N-hydroxysuccinimide to give the succinate II (R1 = OR2, R2 = succinimido).

IC ICM C07D043-02
ICS C07D241-04

INCL 544182000; 544372000; 544209000; 544371000; 544399000

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 856187-87-6P 856187-98-9P 856188-02-8P 856188-06-2P **856188-16-4P 856188-20-0P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)

IT 658-78-6 920-66-1 1737-40-2 4530-20-5, N-Boc-glycine 5672-86-6 5672-89-9 13200-60-7, Sarcosine, ethyl ester 14533-84-7 34352-59-5 54699-92-2 61898-49-5 85539-84-0 856187-95-6 **856188-13-1** 856188-80-2 856188-88-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)

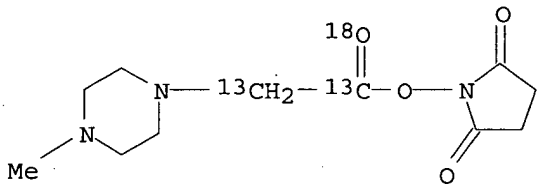
IT 109-01-3P, N-Methylpiperazine 5625-52-5P 145590-97-2P 856187-53-6P 856187-57-0P **856187-64-9P 856187-68-3P 856187-72-9P** 856187-80-9P 856187-83-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)

IT **856187-76-3P 856187-92-3P** 856188-23-3P 856188-27-7P 856188-32-4P 856188-38-0P 856188-44-8P 856188-50-6P 856188-62-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of active esters of N-substituted piperazine acetic acids and

their labeled derivs.)

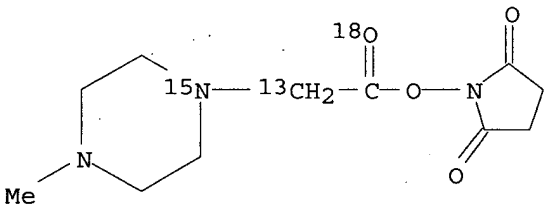
IT **856188-16-4P 856188-20-0P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)

RN 856188-16-4 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-13C2-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

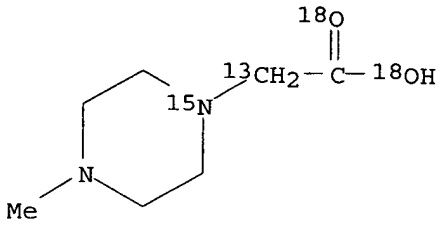
RN 856188-20-0 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl-1-15N)acetyl-2-13C-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

IT **856188-13-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)

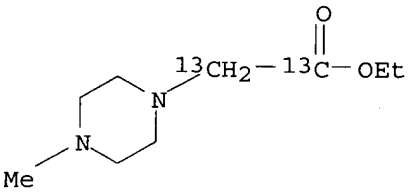
RN 856188-13-1 HCAPLUS
CN 1-Piperazineacetic-α-13C-1-15N-18O2 acid, 4-methyl-, dihydrochloride (9CI) (CA INDEX NAME)



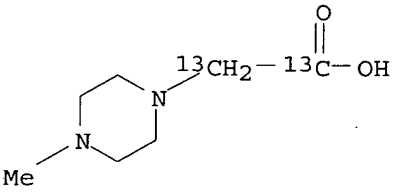
●2 HCl

IT **856187-64-9P 856187-68-3P 856187-72-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)

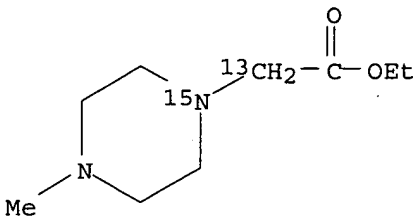
RN 856187-64-9 HCAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2 acid, 4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



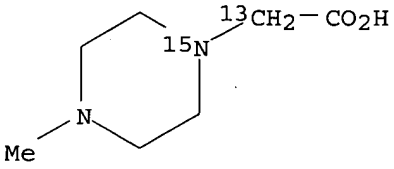
RN 856187-68-3 HCAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2 acid, 4-methyl- (9CI) (CA INDEX NAME)



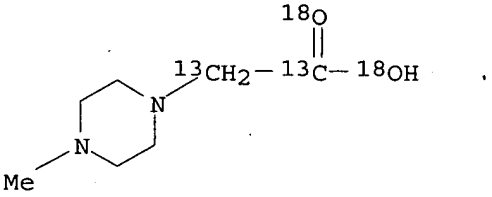
RN 856187-72-9 HCAPLUS
CN 1-Piperazine-1-15N-acetic-α-13C acid, 4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



IT **856187-76-3P 856187-92-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)
RN 856187-76-3 HCAPLUS
CN 1-Piperazine-1-15N-acetic-α-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 856187-92-3 HCAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2-18O2 acid, 4-methyl-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

L92 ANSWER 4 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 4
ACCESSION NUMBER: 2005:588349 HCAPLUS
DOCUMENT NUMBER: 143:112150
TITLE: Isobarically labeled analytes and fragment ions derived therefrom
INVENTOR(S): **Pappin, Darryl J. C.; Purkayastha, Subhasish; Coull, James M.**
PATENT ASSIGNEE(S): Applera Corporation, USA
SOURCE: U.S. Pat. Appl. Publ., 88 pp., Cont.-in-part of U.S. Ser. No. 822,639.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005148087	A1	20050707	US 2004-852730	20040524
US 2005147982	A1	20050707	US 2004-751353	20040105
US 2005147985	A1	20050707	US 2004-822639	20040412
WO 2005068446	A1	20050728	WO 2005-US223	20050105

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

US 2004-751353	A2	20040105
US 2004-822639	A2	20040412
US 2004-751354	A	20040105
US 2004-751387	A	20040105
US 2004-751388	A	20040105
US 2004-852730	A	20040524

OTHER SOURCE(S): MARPAT 143:112150

AB This invention pertains to isobarically labeled analytes and fragment ions thereof.

IC ICM C07K014-47
ICS C12Q001-68; G01N033-00

INCL 436086000; 530409000

CC 9-16 (Biochemical Methods)

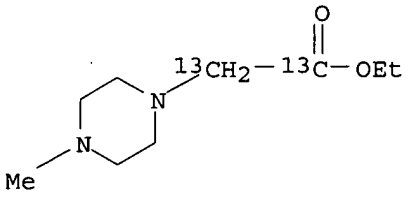
IT 79-08-3DP, Bromoacetic acid, polystyrene trityl chloride piperazine derivs. 110-85-0DP, Piperazine, trityl chloride/bromoacetic polystyrene derivs. 3235-67-4P, 1-Piperidineacetic acid 3235-69-6P, 4-Morpholineacetic acid 5625-52-5P 37478-58-3P, 1-Piperazineacetic acid 53788-49-1P 80841-13-0P 174311-10-5P 215101-76-1P 741683-82-9P, 1-Piperidineacetic-carboxy-13C acid 741683-83-0P, 1-Piperidineacetic-α-13C acid 741683-84-1P, 1-Piperazineacetic-carboxy-13C acid 741683-85-2P, 1-Piperazineacetic-α-13C acid **856187-64-9P 856187-72-9P** 856187-80-9P 856187-83-2P 857027-04-4P 857027-05-5P 857027-07-7P 857027-09-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(isobarically labeled analytes and fragment ions derived therefrom)

IT 109-01-3P 34352-59-5P 741683-79-4P 741683-81-8P 856187-57-0P **856187-68-3P 856187-76-3P** 856187-87-6P 856187-98-9P 856188-06-2P 856188-62-0P **856290-53-4P 856290-55-6P** **857027-06-6P** 857027-08-8P 857027-10-2P **857291-36-2P** **857291-38-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(isobarically labeled analytes and fragment ions derived therefrom)

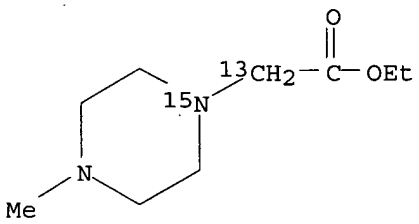
IT **856187-64-9P 856187-72-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(isobarically labeled analytes and fragment ions derived therefrom)

RN 856187-64-9 HCAPLUS

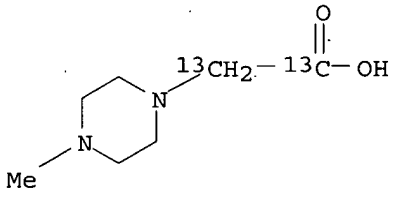
CN 1-Piperazineacetic-carboxy,α-13C2 acid, 4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



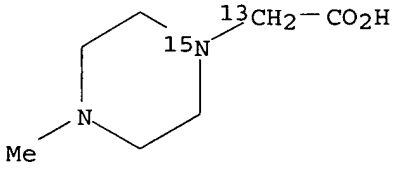
RN 856187-72-9 HCAPLUS
CN 1-Piperazine-1-15N-acetic-α-13C acid, 4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



IT **856187-68-3P 856187-76-3P 856290-53-4P 856290-55-6P 857027-06-6P 857291-36-2P 857291-38-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(isobarically labeled analytes and fragment ions derived therefrom)
RN 856187-68-3 HCAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2 acid, 4-methyl- (9CI) (CA INDEX NAME)

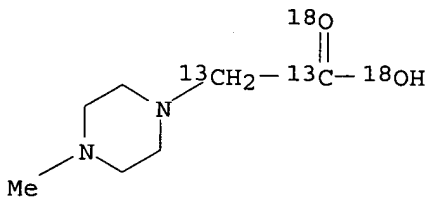


RN 856187-76-3 HCAPLUS
CN 1-Piperazine-1-15N-acetic-α-13C acid, 4-methyl- (9CI) (CA INDEX NAME)

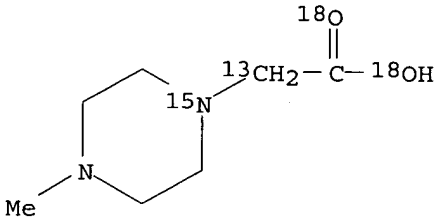


RN 856290-53-4 HCAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2-18O2 acid, 4-methyl- (9CI) (CA

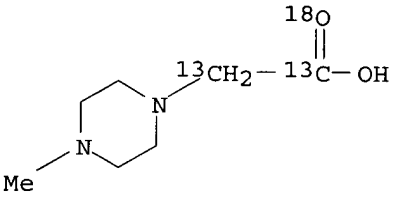
INDEX NAME)



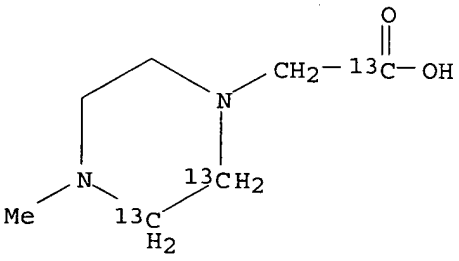
RN 856290-55-6 HCAPLUS
CN 1-Piperazineacetic-α-13C-1-15N-18O2 acid, 4-methyl- (9CI) (CA INDEX NAME)



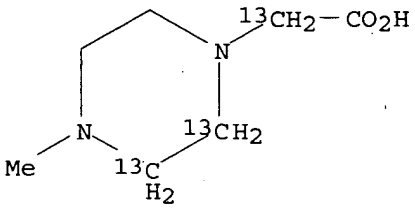
RN 857027-06-6 HCAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2-18O acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 857291-36-2 HCAPLUS
CN 1-Piperazine-2,3-13C2-acetic-carboxy-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 857291-38-4 HCAPLUS
CN 1-Piperazine-2,3-13C2-acetic-α-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



L92 ANSWER 5 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 5
ACCESSION NUMBER: 2005:592027 HCAPLUS
DOCUMENT NUMBER: 143:93642
TITLE: Mixtures of isobarically labeled analytes and fragments ions derived therefrom
INVENTOR(S): **Pappin, Darryl J. C.; Purkayastha, Subhasish; Coull, James M.**
PATENT ASSIGNEE(S): Applera Corp., USA
SOURCE: U.S. Pat. Appl. Publ., 36 pp., Cont.-in-part of U.S. Ser. No. 751,353.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005147985	A1	20050707	US 2004-822639	20040412
US 2005147982	A1	20050707	US 2004-751353	20040105
US 2005148087	A1	20050707	US 2004-852730	20040524
WO 2005068446	A1	20050728	WO 2005-US223	20050105

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

US 2004-751353	A2	20040105
US 2004-751354	A	20040105
US 2004-751387	A	20040105
US 2004-751388	A	20040105
US 2004-822639	A2	20040412
US 2004-852730	A	20040524

OTHER SOURCE(S): MARPAT 143:93642
AB This invention pertains to mixts. of isobarically labeled analytes and fragment ions thereof.
IC ICM C12Q001-68
ICS C07H021-02; G01N033-00; C07J043-00
INCL 435006000; 436086000; 530409000; 536023100; 540107000; 544359000
CC 9-16 (Biochemical Methods)
IT **856290-53-4P 856290-55-6P 857027-11-3P 857027-12-4P**

RL: FMU (Formation, unclassified); SPN (Synthetic preparation); FORM (Formation, nonpreparative); PREP (Preparation)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

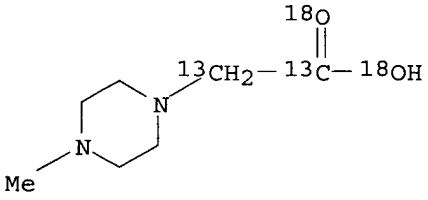
IT 75-89-8 79-08-3, Bromoacetic acid 79-37-8, Ethanedioyl dichloride 139-02-6 771-61-9, Pentafluorophenol 920-66-1 4530-20-5, Boc-Glycine 5672-89-9 6066-82-6 7087-68-5, Diisopropylethylamine 13200-60-7, Sarcosine ethyl ester 18156-74-6 52928-63-9 54699-92-2 56522-24-8 61898-49-5 85539-84-0 99542-20-8 **856187-92-3** 856187-95-6 **856188-13-1** 857027-03-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

IT 5625-52-5P 53788-49-1P 80841-13-0P 145590-97-2P **856187-64-9P** **856187-68-3P** **856187-72-9P** 856187-80-9P 856187-83-2P 856188-06-2P 857027-04-4P 857027-05-5P 857027-07-7P 857027-09-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

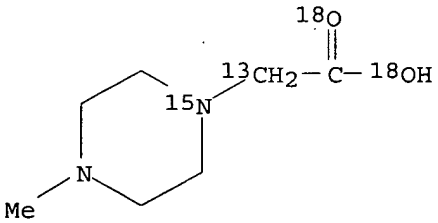
IT 109-01-3P 34352-59-5P 856187-57-0P **856187-76-3P** 856187-87-6P 856187-98-9P **856188-16-4P** **856188-20-0P** 856188-62-0P **857027-06-6DP**, salts 857027-08-8P 857027-10-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

IT **856290-53-4P** **856290-55-6P** **857027-11-3P** **857027-12-4P**
RL: FMU (Formation, unclassified); SPN (Synthetic preparation); FORM (Formation, nonpreparative); PREP (Preparation)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

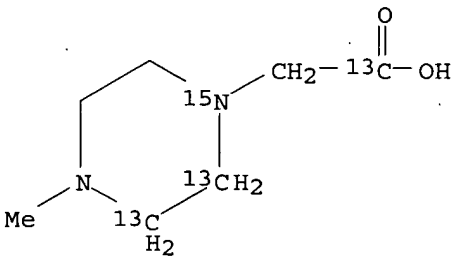
RN 856290-53-4 HCAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2-18O2 acid, 4-methyl- (9CI) (CA INDEX NAME)



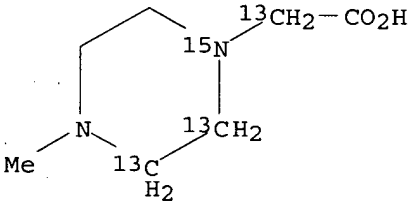
RN 856290-55-6 HCAPLUS
CN 1-Piperazineacetic-α-13C-1-15N-18O2 acid, 4-methyl- (9CI) (CA INDEX NAME)



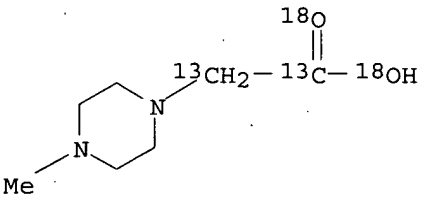
RN 857027-11-3 HCAPLUS
CN 1-Piperazine-2,3-13C2-1-15N-acetic-carboxy-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 857027-12-4 HCAPLUS
CN 1-Piperazine-2,3-13C2-1-15N-acetic-α-13C acid, 4-methyl- (9CI) (CA INDEX NAME)

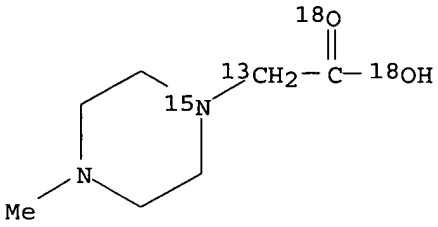


IT **856187-92-3 856188-13-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)
RN 856187-92-3 HCAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2-18O2 acid, 4-methyl-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

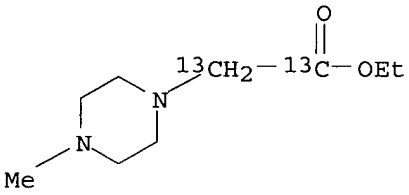
RN 856188-13-1 HCAPLUS
CN 1-Piperazineacetic-α-13C-1-15N-18O2 acid, 4-methyl-, dihydrochloride (9CI) (CA INDEX NAME)



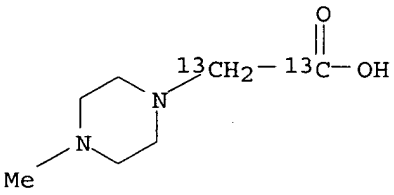
● 2 HCl

IT **856187-64-9P 856187-68-3P 856187-72-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

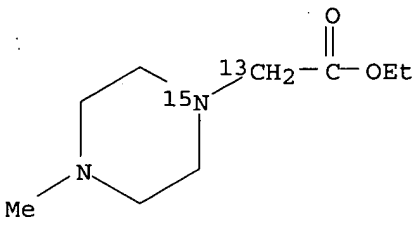
RN 856187-64-9 HCAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2 acid, 4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 856187-68-3 HCAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2 acid, 4-methyl- (9CI) (CA INDEX NAME)

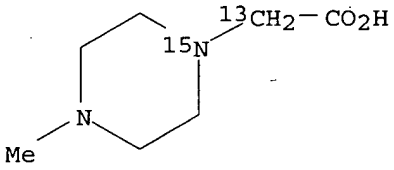


RN 856187-72-9 HCAPLUS
CN 1-Piperazine-1-15N-acetic-α-13C acid, 4-methyl-, ethyl ester (9CI) (CA INDEX NAME)

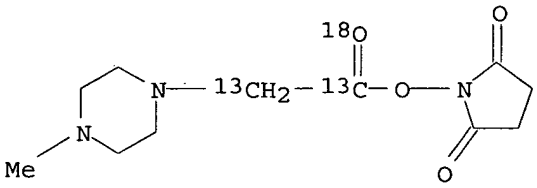


IT **856187-76-3P 856188-16-4P 856188-20-0P**
857027-06-6DP, salts
RL: SPN (Synthetic preparation); PREP (Preparation)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

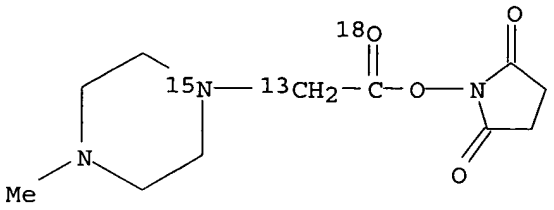
RN 856187-76-3 HCAPLUS
CN 1-Piperazine-1-15N-acetic-α-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 856188-16-4 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-13C2-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)

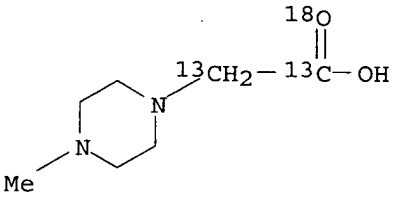


RN 856188-20-0 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl-1-15N)acetyl-2-13C-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 857027-06-6 HCAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2-18O acid, 4-methyl- (9CI) (CA INDEX NAME)



L92 ANSWER 6 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 6
ACCESSION NUMBER: 2005:588336 HCAPLUS
DOCUMENT NUMBER: 143:93635
TITLE: Mixtures of isobarically labeled analytes and fragments ions derived therefrom
INVENTOR(S): **Pappin, Darryl J. C.; Purkayastha, Subhasish; Coull, James M.**
PATENT ASSIGNEE(S): Applera Corporation, USA
SOURCE: U.S. Pat. Appl. Publ., 29 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005147982	A1	20050707	US 2004-751353	20040105
US 2005147985	A1	20050707	US 2004-822639	20040412
US 2005148087	A1	20050707	US 2004-852730	20040524
WO 2005068446	A1	20050728	WO 2005-US223	20050105

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,

RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

US 2004-751353	A2	20040105
US 2004-751354	A	20040105
US 2004-751387	A	20040105
US 2004-751388	A	20040105
US 2004-822639	A2	20040412
US 2004-852730	A	20040524

AB This invention pertains to mixts. of isobarically labeled analytes and fragment ions thereof.

IC ICM C12Q001-68
ICS C07H021-04; G01N033-00; C07K014-47

INCL 435006000; 436086000; 530409000; 536023100

CC 9-16 (Biochemical Methods)

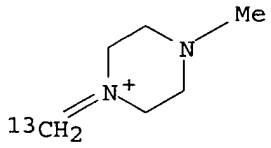
IT **853995-47-8 853995-48-9 853995-49-0**
853995-50-3
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

IT 5625-52-5P 53788-49-1P 61898-49-5P, Ethyl bromoacetate 80841-13-0P
145590-97-2P **856187-64-9P 856187-68-3P**
856187-72-9P 856187-80-9P 856187-83-2P 856188-06-2P
857027-02-2P 857027-04-4P 857027-05-5P 857027-09-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

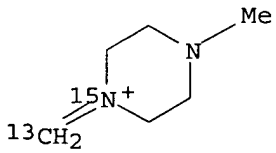
IT 109-01-3P 34352-59-5P 856187-57-0P **856187-76-3P**
856187-87-6P 856187-98-9P 856188-62-0P **856290-53-4P**
856290-55-6P 857027-06-6DP, salts 857027-08-8P
857027-10-2P **857027-11-3P 857027-12-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

IT **853995-47-8 853995-48-9 853995-49-0**
853995-50-3
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

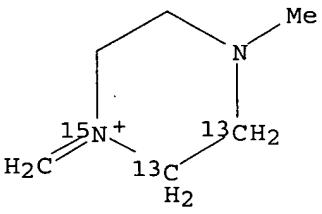
RN 853995-47-8 HCAPLUS
CN Piperazinium, 4-methyl-1-(methylene-13C)- (9CI) (CA INDEX NAME)



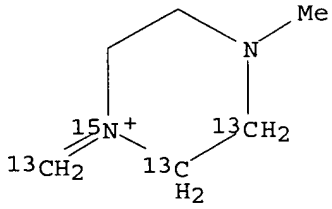
RN 853995-48-9 HCAPLUS
CN Piperazinium-1-15N, 4-methyl-1-(methylene-13C)- (9CI) (CA INDEX NAME)



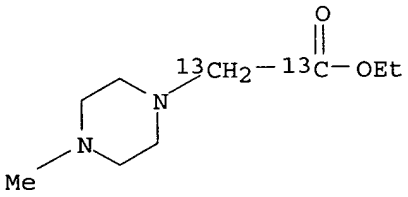
RN 853995-49-0 HCAPLUS
CN Piperazinium-2,3-13C2-1-15N, 4-methyl-1-methylene- (9CI) (CA INDEX NAME)



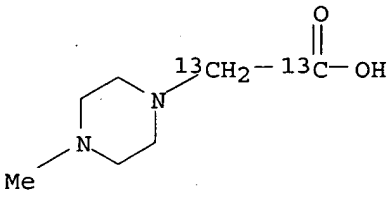
RN 853995-50-3 HCAPLUS
CN Piperazinium-2,3-13C2-1-15N, 4-methyl-1-(methylene-13C)- (9CI) (CA INDEX NAME)



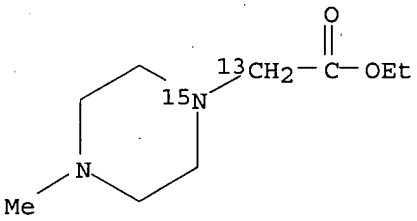
IT **856187-64-9P 856187-68-3P 856187-72-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)
RN 856187-64-9 HCAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2 acid, 4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



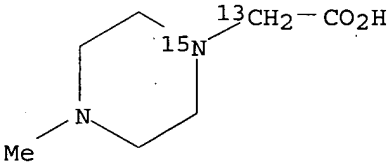
RN 856187-68-3 HCAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2 acid, 4-methyl- (9CI) (CA INDEX NAME)



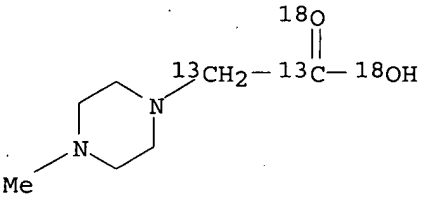
RN 856187-72-9 HCAPLUS
CN 1-Piperazine-1-15N-acetic-α-13C acid, 4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



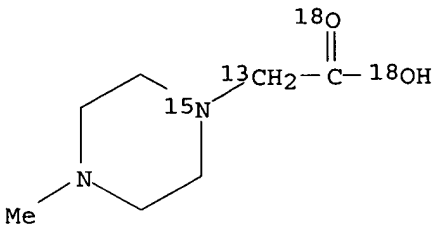
IT **856187-76-3P 856290-53-4P 856290-55-6P 857027-06-6DP**, salts **857027-11-3P 857027-12-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)
RN 856187-76-3 HCAPLUS
CN 1-Piperazine-1-15N-acetic-α-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



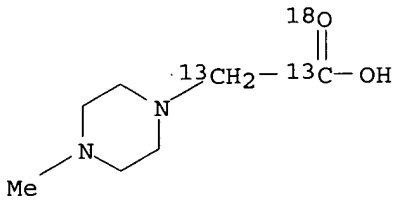
RN 856290-53-4 HCAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2-18O2 acid, 4-methyl- (9CI) (CA INDEX NAME)



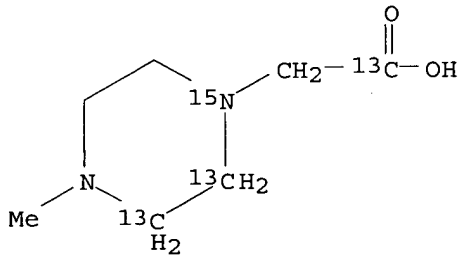
RN 856290-55-6 HCAPLUS
CN 1-Piperazineacetic-α-13C-1-15N-18O2 acid, 4-methyl- (9CI) (CA INDEX NAME)



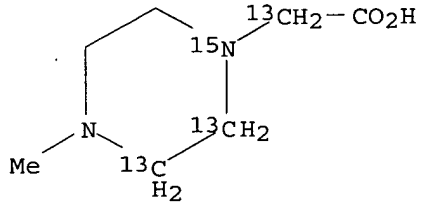
RN 857027-06-6 HCAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2-18O acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 857027-11-3 HCAPLUS
CN 1-Piperazine-2,3-13C2-1-15N-acetic-carboxy-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 857027-12-4 HCAPLUS
CN 1-Piperazine-2,3-13C2-1-15N-acetic-α-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



L92 ANSWER 7 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:371290 HCAPLUS
DOCUMENT NUMBER: 142:409686

TITLE: Method of reducing leachate released in protein A-based affinity purification of antibodies
INVENTOR(S): Leete, Thomas D.; Creasey, Theresa S.; Smith, Robert; **Coull, James M.; Pappin, Darryl J.**; Mccoy, Mark A.
PATENT ASSIGNEE(S): Applera Corporation, USA
SOURCE: PCT Int. Appl., 18 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005037869	A2	20050428	WO 2004-US34249	20041015
WO 2005037869	A3	20050616		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005165222	A1	20050728	US 2004-966188	20041015
PRIORITY APPLN. INFO.:			US 2003-511521P P	20031015

AB The disclosed invention provides methods and compns. used for antibody purification by protein A-based affinity techniques. In particular, methods are provided for reducing the levels of protein A leachate in such affinity-purified antibody prepns. In addition, the present invention relates to protein A affinity chromatog. binding buffer compns. and to antibody compns. In the example, protein A chromatog. was performed using a customized PerSeptive BioCad 700E HPLE system equipped with a stainless steel column (4.6 mm X 10 cm) containing a bed of POROS A50 resin (protein A affinity support from Applied Biosystems). The antibody sample loaded on the equilibrated POROS A50 column is human serum IgG. The inventors also measured the protein A leachate concns. using a protein A ELISA kit, and quantified the protease activity using a suitable enzyme assay.

IC ICM C07K016-06
ICS C07K001-22
CC 15-1 (Immunochemistry)
Section cross-reference(s): 9

L92 ANSWER 8 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:19284 HCAPLUS
DOCUMENT NUMBER: 142:257250
TITLE: Multiplexed protein quantitation in Saccharomyces cerevisiae using amine-reactive isobaric tagging reagents
AUTHOR(S): Ross, Philip L.; Huang, Yulin N.; Marchese, Jason N.; Williamson, Brian; Parker, Kenneth; Hattan, Stephen; Khainovski, Nikita; Pillai, Sasi; Dey, Subhakar; Daniels, Scott; **Purkayastha, Subhasish**; Juhasz, Peter; Martin, Stephen; Bartlet-Jones, Michael; He, Feng; Jacobson, Allan; **Pappin, Darryl J.**

CORPORATE SOURCE: Applied Biosystems, Framingham, MA, 01701, USA
SOURCE: Molecular and Cellular Proteomics (2004), 3(12), 1154-1169
CODEN: MCPOBS; ISSN: 1535-9476
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We describe here a multiplexed protein quantitation strategy that provides relative and absolute measurements of proteins in complex mixts. At the core of this methodol. is a multiplexed set of isobaric reagents that yield amine-derivatized peptides. The derivatized peptides are indistinguishable in MS, but exhibit intense low-mass MS/MS signature ions that support quantitation. In this study, we have examined the global protein expression of a wild-type yeast strain and the isogenic upf1Δ and xrn1Δ mutant strains that are defective in the nonsense-mediated mRNA decay and the general 5' to 3' decay pathways, resp. We also demonstrate the use of 4-fold multiplexing to enable relative protein measurements simultaneously with determination of absolute levels of a target protein using synthetic isobaric peptide stds. We find that inactivation of Upf1p and Xrn1p causes common as well as unique effects on protein expression.

CC 9-16 (Biochemical Methods)
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L92 ANSWER 9 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:425568 HCAPLUS
DOCUMENT NUMBER: 115:25568
TITLE: Immobilization of proteins and peptides on insoluble supports for sequencing and other applications
INVENTOR(S): **Pappin, Darryl J. C.**; **Coull, James M.**; Koester, Hubert
PATENT ASSIGNEE(S): Millipore Corp., USA
SOURCE: Eur. Pat. Appl., 18 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 410323	A2	19910130	EP 1990-113972	19900720
EP 410323	A3	19920408		
R: DE, FR, GB, IT, NL, SE				
US 5071909	A	19911210	US 1989-385711	19890726
JP 03141300	A2	19910617	JP 1990-194113	19900724

PRIORITY APPLN. INFO.: US 1989-385711 A 19890726

AB A peptide or protein is immobilized onto a flat, microporous membrane by (1) adsorbing the peptide or protein and a crosslinkable polymer onto the membrane surface, and (2) crosslinking the polymer to produce a polymer network entrapping the protein or peptide therein. The immobilized peptide or protein is suitable for sequence anal. or other chemical or enzymic processes. Thus, a polyvinylidene difluoride membrane disk containing electroblotted β-lactoglobulin A and stained with sulforhodamine B was treated with diisopropyl-carbodiimide and methylenedianiline (polymer crosslinking agent), dried, then treated with polyacrylic acid (5000 mol. weight). The prepared disk was subjected to 20 cycles of Edman degradation The

initial sequencing yield was 35 pmol and the repetitive yield 90%.
IC ICM G01N033-68
ICA G01N033-549; G01N033-545
CC 9-15 (Biochemical Methods)
Section cross-reference(s): 34

L92 ANSWER 10 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:240863 HCAPLUS
DOCUMENT NUMBER: 114:240863
TITLE: Identification of phosphorylated sites in the mouse glucocorticoid receptor
AUTHOR(S): Bodwell, Jack E.; Orti, Eduardo; **Coull, James M.**; **Pappin, Darryl J. C.**; Smith, Lynda I.; Swift, Fiona
CORPORATE SOURCE: Dep. Physiol., Dartmouth Med. Sch., Hanover, NH, 03756, USA
SOURCE: Journal of Biological Chemistry (1991), 266(12), 7549-55
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Glucocorticoid receptors in vivo are phosphorylated in the absence of hormone and become hyperphosphorylated in the presence of glucocorticoid agonist but not antagonists (Orti, E., et al., 1989). As a preliminary step to elucidating the functional significance of receptor phosphorylation, phosphorylated sites were identified on the mouse receptor. Tryptic phosphopeptides from 32P-labeled receptors were purified from glucocorticoid-treated mouse thymoma cells (WEHI-7) and from stably transfected Chinese hamster ovary cells (WCL2) that express large nos. of mouse receptors. Phosphopeptide maps of receptors from these 2 cell types were almost indistinguishable. Solid phase sequencing revealed phosphorylation at serines 122, 150, 212, 220, 234, and 315 and threonine 159. Serines 122, 150, 212, 220, and 234 and the sequences surrounding them are conserved in the homologous regions of the rat and human receptors, but threonine 159 and serine 315 have no homologues in the human receptor. The 7 phosphorylated sites are in the amino-terminal domain of the receptor. All but serine 315 are within transactivation domains identified in the human and/or rat receptors. Serines 212, 220, and 234 are in a highly acidic region that in the mouse receptor is necessary for full transcription initiation activity and reduces nonspecific DNA binding. Serines 212, 220, and 234 and threonine 159 are in consensus sequences for proline-directed kinase and/or p34cdc2 kinase. Serine 122 is in a consensus sequence for casein kinase II whereas serines 150 and 315 do not appear to be in any known kinase consensus sequence. The location of many of these sites suggests a role of phosphorylation in transactivation.
CC 2-4 (Mammalian Hormones)

L92 ANSWER 11 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:243669 HCAPLUS
DOCUMENT NUMBER: 114:243669
TITLE: Functionalized membrane supports for covalent protein microsequence analysis
AUTHOR(S): **Coull, James M.**; **Pappin, Darryl J. C.**; Mark, Jonathan; Aebersold, Ruedi; Koster, Hubert
CORPORATE SOURCE: MilliGen/Bios., Div. Millipore, Burlington, MA, 01803, USA
SOURCE: Analytical Biochemistry (1991), 194(1), 110-20
CODEN: ANBCA2; ISSN: 0003-2697

DOCUMENT TYPE: Journal
LANGUAGE: English
AB Methods were developed for high-yield covalent attachment of peptides and proteins to isothiocyanate and arylamine-derivatized poly(vinylidene difluoride) membranes for solid-phase sequence anal. Solns. of protein or peptide were dried onto 8-mm membrane disks such that the functional groups on the surface and the polypeptide were brought into close proximity. In the case of the isothiocyanate membrane, reaction between polypeptide amino groups and the surface isothiocyanate moieties was promoted by application of aqueous N-methylmorpholine. Attachment of proteins and peptides to the arylamine surface was achieved by application of water-soluble carbodiimide in a pH 5.0 buffer. Edman degradation of covalently bound polypeptides was accomplished with initial and repetitive sequence yields ranging 33-75% and 88.5-98.5%, resp. The yields were independent of the sample load (20 pmol to >1 nmol) for either surface. Significant loss of material was not observed when attachment residues were encountered during sequence runs. Application of bovine β-lactoglobulin A chain, staphylococcus protein A, or the peptide melittin to the isothiocyanate membrane allowed for extended N-terminal sequence identification (35 residues from 20 pmol of β-lactoglobulin). Several synthetic and naturally occurring peptides were sequenced to the C-terminal residue following attachment to the arylamine surface. In 1 example, 10 μg of bovine α-casein was digested with staphylococcal protease V8 and the peptides were separated by reversed-phase chromatog. Peptide fractions were then directly applied to arylamine membrane disks for covalent sequence anal. From as little as 2 pmol of initial signal it was possible to determine substantial sequence information (>10 residues).
CC 9-3 (Biochemical Methods)

L92 ANSWER 12 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:627543 HCAPLUS
DOCUMENT NUMBER: 113:227543
TITLE: Membranes for solid phase protein sequencing
INVENTOR(S): **Coull, James M.; Pappin, Darryl J. C.**; Koster, Hubert; Pluskal, Malcolm G.; Steuck, Michael J.; Bonner, Alex G.
PATENT ASSIGNEE(S): Millipore Corp., USA
SOURCE: Eur. Pat. Appl., 27 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 353460	A2	19900207	EP 1989-111792	19890628
EP 353460	A3	19910904		
R: DE, FR, GB, IT, NL, SE				
US 5011861	A	19910430	US 1988-212430	19880628
JP 02045537	A2	19900215	JP 1989-164115	19890628
JP 2796599	B2	19980910		

PRIORITY APPLN. INFO.: US 1988-212430 A 19880628
AB A membrane suitable for immobilizing peptides and proteins is disclosed. The membrane is a flexible, polymeric, porous membrane (preferably a polymeric fluorocarbon) which contains functional groups capable of covalently linking peptides and proteins. The functional groups can be provided by reacting the membrane itself or a coating thereon with nucleophiles which provide amino, mercapto, hydroxyl, or carboxyl functionality to the membrane surface. Addnl., surfaces containing amino

groups can be further reacted with diisothiocyanates to provide an isothiocyanate functionality having enhanced covalent binding characteristics. A particularly preferred membrane for protein sequencing is a poly(vinylidene difluoride) membrane coated with crosslinked hydroxypropyl acrylate having isothiocyanate functional groups. The above membrane was prepared by activating a 2-hydroxypropyl acrylate-coated poly(vinylidene difluoride) membrane (DVPP membrane, Millipore) with 1,1'-carbonyl diimidazole, reacting the activated membrane with 1,3-diaminopropane, and then reacting the amino functionalized membrane with 1,3-phenylene diisothiocyanate. Horse heart myoglobin was immobilized on the thus-prepared membrane, and was sequenced in an automated solid-phase sequencer using 30 cycles of Edman degradation (Laursen, R. A.; 1971).

IC ICM C07K017-02
ICS G01N033-68
ICA B01D067-00; B01D069-00
CC 9-2 (Biochemical Methods)
Section cross-reference(s): 35

L92 ANSWER 13 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:467672 HCAPLUS
DOCUMENT NUMBER: 115:67672
TITLE: New approaches to covalent sequence analysis
AUTHOR(S): **Pappin, Darryl J. C.; Coull, James M.**; Koester, Hubert
CORPORATE SOURCE: MilliGen/Biosearch Div., Millipore, Burlington, MA, 01803, USA
SOURCE: Curr. Res. Protein Chem.: Tech., Struct., Funct., [Pap. Annu. Symp. Protein Soc.], 3rd (1990), Meeting Date 1989, 191-202. Editor(s): Villafranca, Joseph J. Academic: San Diego, Calif.
CODEN: 56XQAW
DOCUMENT TYPE: Conference
LANGUAGE: English
AB A symposium report on covalent (solid-phase) sequence anal. of proteins. Thus, peptides or proteins are blotted onto an underivatized polyvinylidene membranes, stained by conventional techniques, and then efficiently covalently immobilized to the membrane surface by entrapment in a thin polymer coating.
CC 9-1 (Biochemical Methods)

L92 ANSWER 14 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:420480 HCAPLUS
DOCUMENT NUMBER: 113:20480
TITLE: Solid-phase sequence analysis of proteins electroblotted or spotted onto polyvinylidene difluoride membranes
AUTHOR(S): **Pappin, Darryl J. C.; Coull, James M.**; Koster, Hubert
CORPORATE SOURCE: MilliGen/Biosearch, Burlington, MA, 01803, USA
SOURCE: Analytical Biochemistry (1990), 187(1), 10-19
CODEN: ANBCA2; ISSN: 0003-2697
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Electroblotted proteins noncovalently bound to polyvinylidene difluoride (PVDF) membranes are typically sequenced using adsorptive sequencer protocols (gas phase or pulsed-liquid) that do not require a covalent linkage between protein and surface. Simple chemical protocols were developed where proteins are first electroblotted onto unmodified PVDF membranes, visualized with common protein stains, and then immobilized for

solid-phase sequence anal. Adsorbed, stained proteins are first treated with phenylisothiocyanate (PITC) to modify α and ε amines. The protein is then overlayed with a solution of 1,4-phenylene diisothiocyanate (DITC), followed by a few microliters of a basic solution containing a poly(alkylamine). As the polymer dries onto the surface both polymer and remaining protein amino groups are crosslinked by DITC. The protein is thus immobilized to the membrane surface by entrapment in a thin polymer coating. The coating is transparent to the degradation chemical, and extensive enough to remain immobilized even in the absence of any covalent link between polymer and surface. Partial modification with PITC allows for identification of N-terminal and internal lysine residues during sequencing. The process was tested with a variety of poly(alkylamines), linear and branched, with mol. wts. ranging from 600 to >100,000. Proteins bound in this manner were successfully sequenced using covalent (solid-phase) sequencer protocols with cyclic times as short as 26 min.

CC 9-15 (Biochemical Methods)

L92 ANSWER 15 OF 16 USPATFULL on STN

ACCESSION NUMBER: 2005:190304 USPATFULL

TITLE: Method of reducing leachate from protein a affinity media

INVENTOR(S): Leete, Thomas D., Westford, MA, UNITED STATES
Creasey, Theresa S., Bedford, MA, UNITED STATES
Smith, Robert M., Stow, MA, UNITED STATES
Coull, James M., Westford, MA, UNITED STATES
Pappin, Darryl J., Boxborough, MA, UNITED STATES
Edwards, Brooks, Cambridge, MA, UNITED STATES
McCoy, Mark A., Framingham, MA, UNITED STATES

PATENT ASSIGNEE(S): Applera Corporation, Foster City, CA, UNITED STATES, 94404 (U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2005165222	A1	20050728	
APPLICATION INFO.:	US 2004-966188	A1	20041015	(10)

	NUMBER	DATE
PRIORITY INFORMATION:	US 2003-511521P	20031015 (60)

DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: MILA KASAN, PATENT DEPT., APPLIED BIOSYSTEMS, 850 LINCOLN CENTRE DRIVE, FOSTER CITY, CA, 94404, US
NUMBER OF CLAIMS: 27
EXEMPLARY CLAIM: 1
LINE COUNT: 608
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Disclosed are methods and compositions that may be used for purifying antibodies.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IN **Coull, James M.**, Westford, MA, UNITED STATES
IN **Pappin, Darryl J.**, Boxborough, MA, UNITED STATES

L92 ANSWER 16 OF 16 USPATFULL on STN

ACCESSION NUMBER: 91:100423 USPATFULL
TITLE: Immobilization of proteins and peptides on insoluble supports
INVENTOR(S): **Pappin, Darryl J. C.**, West Concord, MA, United States
Coull, James M., Acton, MA, United States
Koester, Hubert, Concord, MA, United States
PATENT ASSIGNEE(S): Millipore Corporation, Bedford, MA, United States (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 5071909		19911210
APPLICATION INFO.:	US 1989-385711		19890726 (7)

DOCUMENT TYPE: Utility
FILE SEGMENT: Granted
PRIMARY EXAMINER: Page, Thurman K.
ASSISTANT EXAMINER: Kishori, G. S.
LEGAL REPRESENTATIVE: Hamilton, Brook, Smith & Reynolds
NUMBER OF CLAIMS: 30
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 5 Drawing Figure(s); 3 Drawing Page(s)
LINE COUNT: 807
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention pertains to a method for immobilizing proteins or peptides onto a flat, microporous membrane surface in a form suitable for sequence analysis or other chemical or enzymatic processes. The process involves the formation of a thin polymer network that entraps the protein or peptide therein.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IN **Pappin, Darryl J. C.**, West Concord, MA, United States
IN **Coull, James M.**, Acton, MA, United States

STRUCTURE/TEXT search

=> □

=> file hcaplus
FILE 'HCAPLUS' ENTERED AT 16:03:38 ON 01 MAR 2006
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FILE COVERS 1907 - 1 Mar 2006 VOL 144 ISS 10
FILE LAST UPDATED: 28 Feb 2006 (20060228/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate
substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d que nos L50

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L8              STR
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L18           923 SEA FILE=REGISTRY ABB=ON  PLU=ON  "CARBON-13"
L19          3243 SEA FILE=REGISTRY ABB=ON  PLU=ON  "CARBON-14"
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L33         11153 SEA FILE=HCAPLUS ABB=ON  PLU=ON  NITROGEN 15/OBI
L34         62382 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L32 OR L33
L35            58 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L34 AND L12
L36        428770 SEA FILE=HCAPLUS ABB=ON  PLU=ON  LABEL?/BI
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L40         6125 SEA FILE=HCAPLUS ABB=ON  PLU=ON  N 15/BI
L43        44703 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L3
L46        55408 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CARBON 13/BI
L47        11292 SEA FILE=HCAPLUS ABB=ON  PLU=ON  NITROGEN 15/BI
L48        80814 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L46 OR L47 OR L39 OR L40
L49          109 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L48 AND L43
L60       321506 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ISOTOP?/BI
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=> d que nos L63

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L40         6125 SEA FILE=HCAPLUS ABB=ON  PLU=ON  N 15/BI
L43        44703 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L3
L46        55408 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CARBON 13/BI
L47        11292 SEA FILE=HCAPLUS ABB=ON  PLU=ON  NITROGEN 15/BI
L48        80814 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L46 OR L47 OR L39 OR L40
L49          109 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L48 AND L43
L62        17234 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ISOBAR?/BI
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=> d que nos L65

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L40         6125 SEA FILE=HCAPLUS ABB=ON  PLU=ON  N 15/BI
L43        44703 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L3
L46        55408 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CARBON 13/BI
L47        11292 SEA FILE=HCAPLUS ABB=ON  PLU=ON  NITROGEN 15/BI
L48        80814 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L46 OR L47 OR L39 OR L40
L49          109 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L48 AND L43
L64       392306 SEA FILE=HCAPLUS ABB=ON  PLU=ON  FRAGMENT?/BI
L65            5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L64 AND L49


=> d que nos L54

L1              STR
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L39        12370 SEA FILE=HCAPLUS ABB=ON  PLU=ON  C 13/BI
L40         6125 SEA FILE=HCAPLUS ABB=ON  PLU=ON  N 15/BI
L43        44703 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L3
L46        55408 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CARBON 13/BI
L47        11292 SEA FILE=HCAPLUS ABB=ON  PLU=ON  NITROGEN 15/BI
L48        80814 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L46 OR L47 OR L39 OR L40
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L54            5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L48 AND L43 AND L53
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=> d que nos L75

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L43         44703 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L3
L46         55408 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CARBON 13/BI
L47         11292 SEA FILE=HCAPLUS ABB=ON  PLU=ON  NITROGEN 15/BI
L48         80814 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L46 OR L47 OR L39 OR L40
L49           109 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L48 AND L43
L74           936 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ?LABEL?/BI (L) ?PIPERAZ?/BI
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=> d que nos L79

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L43         44703 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L3
L46         55408 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CARBON 13/BI
L47         11292 SEA FILE=HCAPLUS ABB=ON  PLU=ON  NITROGEN 15/BI
L48         80814 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L46 OR L47 OR L39 OR L40
L49           109 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L48 AND L43
L78            92 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ?ENRICH?/BI (L) ?PIPERAZ?/BI
L79             0 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L78 AND L49


=> s (L50 or L51 or L37 or L61 or L63 or L65 or L54 or L75 or L79) not L90

L93            34 (L50 OR L51 OR L37 OR L61 OR L63 OR L65 OR L54 OR L75 OR L79)
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=> file uspatfull

FILE 'USPATFULL' ENTERED AT 16:03:46 ON 01 MAR 2006
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FILE COVERS 1971 TO PATENT PUBLICATION DATE: 28 Feb 2006 (20060228/PD)
FILE LAST UPDATED: 28 Feb 2006 (20060228/ED)
HIGHEST GRANTED PATENT NUMBER: US7007305
HIGHEST APPLICATION PUBLICATION NUMBER: US2006041984
CA INDEXING IS CURRENT THROUGH 28 Feb 2006 (20060228/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 28 Feb 2006 (20060228/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Dec 2005
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Dec 2005


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L10            55 SEA FILE=REGISTRY SUB=L3 SSS FUL L8
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=> s L86 not L91

L94          5 L86 NOT L91
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CA INDEXING COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)
PROCESSING COMPLETED FOR L93
PROCESSING COMPLETED FOR L94
L95          37 DUP REM L93 L94 (2 DUPLICATES REMOVED)
                ANSWERS '1-34' FROM FILE HCAPLUS
                ANSWERS '35-37' FROM FILE USPATFULL

=> d ibib abs hitind hitstr L95 1-34; d ibib abs kwic hitstr L95 35-37

L95  ANSWER 1 OF 37  HCAPLUS  COPYRIGHT 2006 ACS on STN DUPLICATE 1
ACCESSION NUMBER:         2005:1132612  HCAPLUS
DOCUMENT NUMBER:          143:392950
TITLE:                    Microfluidic apparatus and method for synthesis of
                          molecular imaging probes
INVENTOR(S):              Buchanan, Charles Russell; Padgett, Henry C.; Collier,
                          Thomas Lee
PATENT ASSIGNEE(S):       USA
SOURCE:                   U.S. Pat. Appl. Publ., 24 pp.
                          CODEN: USXXCO
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
     ---------------      ----   --------    --------------------    --------
     US 2005232861         A1    20051020    US 2004-827992          20040420
PRIORITY APPLN. INFO.:                       US 2004-827992          20040420
AB   The invention provides a method and apparatus for preparation of radiochems.
wherein
     the reaction that couples the radioactive isotope to the reactive
     precursor to form a positron-emitting mol. imaging probe is performed in a
     microfluidic environment.  The method comprises: providing a micro
     reactor; introducing a liquid reactive precursor dissolved in a polar
     aprotic solvent into an inlet port of the micro reactor, the reactive
     precursor adapted for reaction with a radioactive isotope to form a
     radiochem.; introducing a solution comprising a radioactive isotope dissolved
     in a polar aprotic solvent into another inlet port of the micro reactor;
     contacting the reactive precursor with the isotope-containing solution in a
     microchannel of the micro reactor; reacting the reactive precursor with
     the isotope-containing solution as the reactive precursor and
isotope-containing
     solution flow through the microchannel of the micro reactor, wherein the
     reacting step is conducted at a temperature above the b.p. of the polar aprotic
     solvent at 1 atm and at a pressure sufficient to maintain the polar
     aprotic solvent in liquid form; and collecting the resulting radiochem. from
     the micro reactor.
IC   ICM  A61K051-00
     ICS  C07F005-00
```
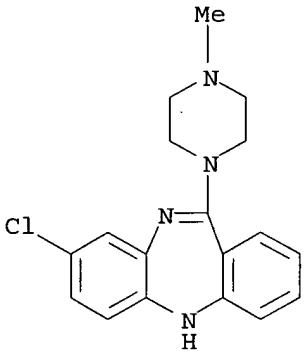

INCL 424001110; 534011000
CC 63-5 (Pharmaceuticals)
Section cross-reference(s): 8
IT 13981-22-1DP, Nitrogen-13, compds., biological studies 13981-56-1DP, Fluorine 18, compds., biological studies 13982-43-9DP, Oxygen 15, compds., biological studies 14158-30-6DP, Iodine 124, compds., biological studies 14333-33-6DP, Carbon 11, compds., biological studies 58576-49-1P, biological studies 63503-12-8P 67829-10-1P 92812-82-3P 94153-50-1P 94793-58-5P 97849-54-2P 98253-49-7P 104613-87-8P 105285-83-4P 107340-59-0P 118931-16-1P, Thymidine-11C 121513-12-0P 128592-98-3P 138558-72-2P 168010-57-9P 183892-17-3P 187671-70-1P 188779-41-1P 206067-82-5P 287114-80-1P 590365-47-2P
786652-70-8P 786652-76-4P
RL: DGN (Diagnostic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(microfluidic apparatus and method for synthesis of mol. imaging probes)
IT **786652-70-8P**
RL: DGN (Diagnostic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(microfluidic apparatus and method for synthesis of mol. imaging probes)
RN 786652-70-8 HCAPLUS
CN 5H-Dibenzo[b,e][1,4]diazepine, 8-chloro-11-(4-methyl-1-piperazinyl)-, labeled with carbon-11 (9CI) (CA INDEX NAME)



L95 ANSWER 2 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 2005:1132582 HCAPLUS
DOCUMENT NUMBER: 143:392949
TITLE: Microfluidic apparatus and method for synthesis of molecular imaging probes
INVENTOR(S): Padgett, Henry C.; Buchanan, Charles Russell; Collier, Thomas Lee; Matteo, Joseph C.; Alvord, Charles W.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 22 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005232387	A1	20051020	US 2004-827893	20040420
PRIORITY APPLN. INFO.:			US 2004-827893	20040420

AB The invention provides a method and apparatus for preparation of radiochems., such as PET mol. imaging probes, wherein the reaction step or steps that couple the radioactive isotope to an organic or inorg. compound to form a positron-emitting mol. imaging probe are performed in a microfluidic environment. The method for synthesizing a radiochem. in a microfluidic environment comprises: i) providing a micro reactor comprising a first inlet port, a second inlet port, an outlet port, and at least one microchannel in fluid communication with the first and second inlet ports and the outlet port; ii) introducing a reactive precursor into the first inlet port of the micro reactor, the reactive precursor adapted for reaction with a radioactive isotope to form a radiochem.; iii) introducing a solution comprising a radioactive isotope into the second inlet port of the micro reactor; iv) contacting the reactive precursor with the isotope-containing solution in the microchannel of the micro reactor; v) reacting the reactive precursor with the isotope-containing solution as the reactive precursor and isotope-containing solution flow through the microchannel of the micro reactor, the reacting step resulting in formation of a radiochem.; and vi) collecting the radiochem. from the outlet port of the micro reactor.

IC ICM A61M036-14

INCL 376194000

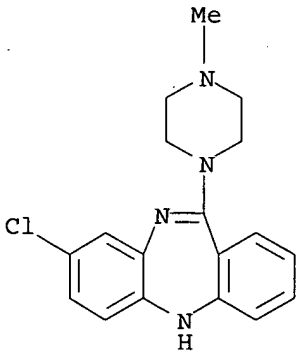
CC 63-5 (Pharmaceuticals)
Section cross-reference(s): 8, 47, 71

IT 58576-49-1P, biological studies 63503-12-8P 67829-10-1P 92812-82-3P 94153-50-1P 94793-58-5P 97849-54-2P 98253-49-7P 104613-87-8P 105285-83-4P 107340-59-0P 118931-16-1P, Thymidine-11C 121513-12-0P 128592-98-3P 138558-72-2P 168010-57-9P 183892-17-3P 187671-70-1P 188779-41-1P 206067-82-5P 287114-80-1P 590365-47-2P **786652-70-8P** 786652-76-4P
RL: DGN (Diagnostic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(microfluidic apparatus for synthesis of mol. imaging probes)

IT **786652-70-8P**
RL: DGN (Diagnostic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(microfluidic apparatus for synthesis of mol. imaging probes)

RN 786652-70-8 HCAPLUS

CN 5H-Dibenzo[b,e][1,4]diazepine, 8-chloro-11-(4-methyl-1-piperazinyl)-, labeled with carbon-11 (9CI) (CA INDEX NAME)



L95 ANSWER 3 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:523758 HCAPLUS
DOCUMENT NUMBER: 143:56140
TITLE: Analysis of mass spectral data in the quiet zones using **label fragment** ions and applications in analysis of proteins and other biomolecules
INVENTOR(S): Pappin, Darryl J. C.
PATENT ASSIGNEE(S): Applera Corporation, USA
SOURCE: PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005054871	A2	20050616	WO 2004-US41343	20041124
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005153456	A1	20050714	US 2004-999638	20041126
PRIORITY APPLN. INFO.:			US 2003-525478P P	20031126
			US 2004-547375P P	20040224

OTHER SOURCE(S): MARPAT 143:56140

AB The invention pertains to methods, systems and/or compns. useful for the anal. of **labels** and/or **labeled** analytes in quiet zones. Because the **labeling** reagents can be **isotopically enriched, label fragment** ions generated by **fragmentation** of a **label** in a mass spectrometer can produce an **isotopic** cluster of distinct peak configuration. The **labeling** reagents that **fragment** to produce the **isotopic** clusters observed in the mass spectrum can be directed to "quiet zones" across a mass spectrum. The "quiet zones" are areas where little or no mass intensity information exists in the summed result for the analyte type or types. By directing the anal. to the quiet zones, where few or no analyte **fragment** ions are detected, it is possible to improve the reliability of any qual. and/or quant. anal. of the **label** based on determination of the **label fragment** ions. The method can be used for mass spectrometric anal. of proteins, peptides, lipids, nucleic acids, carbohydrates or small mols.

IC ICM G01N033-68
ICS C07D211-40; C07D211-10; C07D211-56; C07F009-00; C07D265-00; C07D279-00; C07D217-00
CC 9-5 (Biochemical Methods)
ST mass spectra quiet zone **isotope label fragmentation** protein biomol
IT Collision-induced dissociation
Fragmentation reaction
Ions
Isotope indicators
Mass spectra

Mass spectrometry
(anal. of mass spectral data in quiet zones using **label fragment** ions and applications in anal. of proteins and other biomols.)

IT Biochemical compounds
Carbohydrates, analysis
Lipids, analysis
Nucleic acids
Peptide nucleic acids
Peptides, analysis
Proteins
RL: ANT (Analyte); ANST (Analytical study)
(anal. of mass spectral data in quiet zones using **label fragment** ions and applications in anal. of proteins and other biomols.)

IT Energy
(dissociative; anal. of mass spectral data in quiet zones using **label fragment** ions and applications in anal. of proteins and other biomols.)

IT **Isotopes**
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(heavy; anal. of mass spectral data in quiet zones using **label fragment** ions and applications in anal. of proteins and other biomols.)

IT Clusters
(**isotopic**; anal. of mass spectral data in quiet zones using **label fragment** ions and applications in anal. of proteins and other biomols.)

IT Molecules
(small; anal. of mass spectral data in quiet zones using **label fragment** ions and applications in anal. of proteins and other biomols.)

IT **853995-43-4 853995-44-5 853995-45-6**
853995-46-7
RL: ARG (Analytical reagent use); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent); USES (Uses)
(anal. of mass spectral data in quiet zones using **label fragment** ions and applications in anal. of proteins and other biomols.)

IT 110-85-0D, **Piperazine**, compds. 110-89-4D, Piperidine, compds. 110-91-8D, Morpholine, compds.
RL: ARG (Analytical reagent use); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent); USES (Uses)
(**fragmentation** of; anal. of mass spectral data in quiet zones using **label fragment** ions and applications in anal. of proteins and other biomols.)

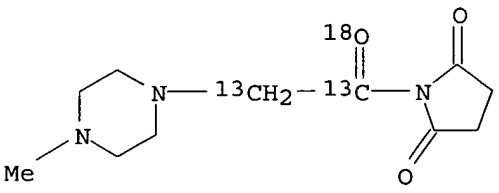
IT 7782-39-0, Deuterium, uses 13981-73-2, Chlorine-37, uses 14380-59-7, Bromine-81, uses 14390-96-6, **Nitrogen-15**, uses 14762-74-4, **Carbon-13**, uses 14797-71-8, Oxygen-18, uses
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(**isotope label**; anal. of mass spectral data in quiet zones using **label fragment** ions and applications in anal. of proteins and other biomols.)

IT **853995-47-8P 853995-48-9P 853995-49-0P**
853995-50-3P
RL: ARG (Analytical reagent use); PNU (Preparation, unclassified); ANST (Analytical study); PREP (Preparation); USES (Uses)
(**label fragment** ion; anal. of mass spectral data in quiet zones using **label fragment** ions and

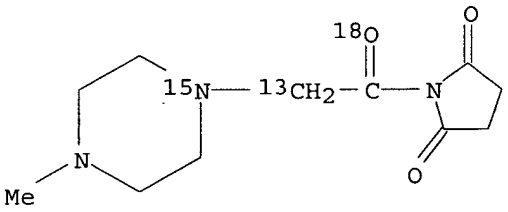
applications in anal. of proteins and other biomols.)

IT **853995-43-4 853995-44-5 853995-45-6 853995-46-7**
RL: ARG (Analytical reagent use); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent); USES (Uses)
(anal. of mass spectral data in quiet zones using **label fragment** ions and applications in anal. of proteins and other biomols.)

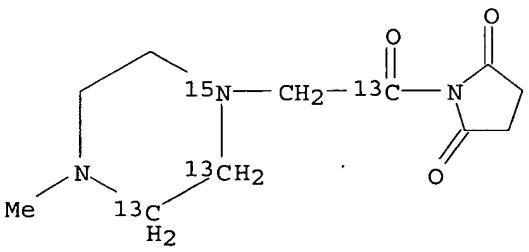
RN 853995-43-4 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[(4-methyl-1-piperazinyl)acetyl-13C2-18O]- (9CI) (CA INDEX NAME)



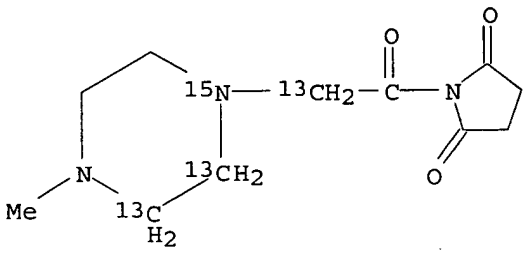
RN 853995-44-5 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[(4-methyl-1-piperazinyl-1-15N)acetyl-2-13C-18O]- (9CI) (CA INDEX NAME)



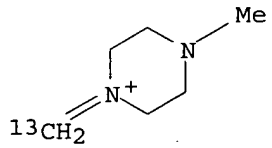
RN 853995-45-6 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[(4-methyl-1-piperazinyl-2,3-13C2-1-15N)acetyl-1-13C]- (9CI) (CA INDEX NAME)



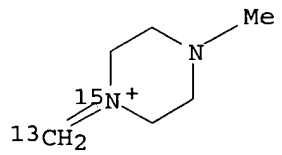
RN 853995-46-7 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[(4-methyl-1-piperazinyl-2,3-13C2-1-15N)acetyl-2-13C]- (9CI) (CA INDEX NAME)



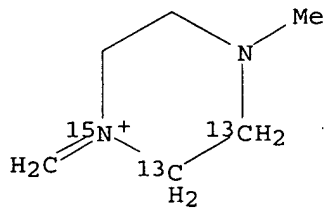
IT **853995-47-8P 853995-48-9P 853995-49-0P**
853995-50-3P
RL: ARG (Analytical reagent use); PNU (Preparation, unclassified); ANST (Analytical study); PREP (Preparation); USES (Uses)
(**label fragment** ion; anal. of mass spectral data in quiet zones using **label fragment** ions and applications in anal. of proteins and other biomols.)
RN 853995-47-8 HCAPLUS
CN Piperazinium, 4-methyl-1-(methylene-13C)- (9CI) (CA INDEX NAME)



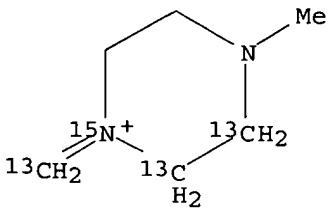
RN 853995-48-9 HCAPLUS
CN Piperazinium-1-15N, 4-methyl-1-(methylene-13C)- (9CI) (CA INDEX NAME)



RN 853995-49-0 HCAPLUS
CN Piperazinium-2,3-13C2-1-15N, 4-methyl-1-methylene- (9CI) (CA INDEX NAME)



RN 853995-50-3 HCAPLUS
CN Piperazinium-2,3-13C2-1-15N, 4-methyl-1-(methylene-13C)- (9CI) (CA INDEX NAME)



L95 ANSWER 4 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:926988 HCAPLUS
DOCUMENT NUMBER: 141:400874
TITLE: System and method for synthesis of molecular imaging probes including FDG
INVENTOR(S): Buchanan, Charles R.; Padgett, Henry C.; Collier, Thomas L.; Matteo, Joseph C.; Alvord, C. William
PATENT ASSIGNEE(S): Molecular Technologies, Inc., USA
SOURCE: PCT Int. Appl., 56 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004093652	A2	20041104	WO 2004-US12189	20040420
WO 2004093652	A3	20050526		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2523189	AA	20041104	CA 2004-2523189	20040420
US 2004258615	A1	20041223	US 2004-827991	20040420
US 2004262158	A1	20041230	US 2004-828844	20040421
PRIORITY APPLN. INFO.:			US 2003-464424P P	20030422
			WO 2004-US12189 W	20040420

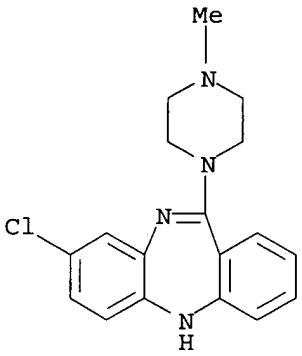
AB The invention provides a method and apparatus for preparation of radiochems. wherein the reaction that couples the radioactive isotope to the reactive precursor to form a positron-emitting mol. imaging probe is performed in a microfluidic environment. Examples are provided of the preparation of 2-deoxy-2-[18F]fluoro-D-glucose.
IC ICM A61B
CC 63-5 (Pharmaceuticals)
Section cross-reference(s): 8
IT 13981-22-1D, Nitrogen 13, compds., biological studies 13981-56-1D, Fluorine 18, compds., biological studies 13982-43-9D, Oxygen 15, compds., biological studies 14158-30-6D, Iodine 124, compds., biological studies 14333-33-6D, Carbon 11, compds., biological studies 58576-49-1, biological studies 67829-10-1, 5-[18F]Fluoro-2'-deoxyuridine

94153-50-1, [11C]-N-Methylspiperone 97849-54-2 98253-49-7
104613-87-8, [18F]Fluoromisonidazole 107340-59-0 121513-12-0
124705-15-3 138558-72-2 168010-57-9, [11C]-Cocaine 183892-17-3
187671-70-1 206067-82-5 259738-99-3 287114-80-1 **786652-70-8**
786652-72-0 786652-74-2, biological studies 786652-76-4
RL: DGN (Diagnostic use); BIOL (Biological study); USES (Uses)
(synthesis of radiol. imaging agents in microfluidic reactors)

IT **786652-70-8**
RL: DGN (Diagnostic use); BIOL (Biological study); USES (Uses)
(synthesis of radiol. imaging agents in microfluidic reactors)

RN 786652-70-8 HCAPLUS

CN 5H-Dibenzo[b,e][1,4]diazepine, 8-chloro-11-(4-methyl-1-piperazinyl)-, labeled with carbon-11 (9CI) (CA INDEX NAME)



L95 ANSWER 5 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:566909 HCAPLUS

DOCUMENT NUMBER: 141:256743

TITLE: Screening Molecular Associations with Lipid Membranes Using Natural Abundance 13C Cross-Polarization Magic-Angle Spinning NMR and Principal Component Analysis

AUTHOR(S): Middleton, David A.; Hughes, Eleri; Madine, Jillian

CORPORATE SOURCE: Department of Biomolecular Sciences, University of Manchester Institute of Science and Technology, Manchester, M60 1QD, UK

SOURCE: Journal of the American Chemical Society (2004), 126(31), 9478-9479
CODEN: JACSAT; ISSN: 0002-7863

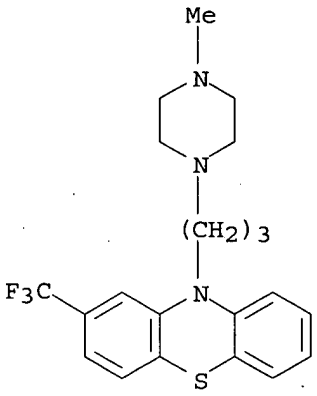
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We describe an NMR approach for detecting the interactions between phospholipid membranes and proteins, peptides, or small mols. First, 1H-13C dipolar coupling profiles are obtained from hydrated lipid samples at natural **isotope** abundance using cross-polarization magic-angle spinning NMR methods. Principal component anal. of dipolar coupling profiles for synthetic lipid membranes in the presence of a range of biol. active additives reveals clusters that relate to different modes of interaction of the additives with the lipid bilayer. Finally, by representing profiles from multiple samples in the form of contour plots, it is possible to reveal statistically significant changes in dipolar couplings, which reflect perturbations in the lipid mols. at the membrane surface or within the hydrophobic interior.

CC 9-5 (Biochemical Methods)
Section cross-reference(s): 6, 80
IT Protein motifs
(IgG binding domain of protein G; peptides, proteins and small mols. exhibit quite distinct modes of association with lipid membrane as determine by
carbon-13 CP-MAS NMR and principal component anal.)
IT Proteins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(IgG-binding, G; peptides, proteins and small mols. exhibit quite distinct modes of association with lipid membrane as determine by **carbon-13** CP-MAS NMR and principal component anal.)
IT Membrane, biological
(bilayer, phospholipid; peptides, proteins and small mols. exhibit quite distinct modes of association with lipid membrane as determine by **carbon-13** CP-MAS NMR and principal component anal.)
IT MAS NMR spectroscopy
(**carbon-13**, CP; peptides, proteins and small mols. exhibit quite distinct modes of association with lipid membrane as determine by
carbon-13 CP-MAS NMR and principal component anal.)
IT Hydrophobicity
Molecular association
Nuclear spin-spin coupling
Principal component analysis
(peptides, proteins and small mols. exhibit quite distinct modes of association with lipid membrane as determine by **carbon-13** CP-MAS NMR and principal component anal.)
IT Peptides, biological studies
Phospholambans
Phospholipids, biological studies
Proteins
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(peptides, proteins and small mols. exhibit quite distinct modes of association with lipid membrane as determine by **carbon-13** CP-MAS NMR and principal component anal.)
IT **117-89-5**, Trifluoperazine 18656-38-7, Dimyristoylphosphatidylcholine 21743-35-1
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(peptides, proteins and small mols. exhibit quite distinct modes of association with lipid membrane as determine by **carbon-13** CP-MAS NMR and principal component anal.)
IT **117-89-5**, Trifluoperazine
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(peptides, proteins and small mols. exhibit quite distinct modes of association with lipid membrane as determine by **carbon-13** CP-MAS NMR and principal component anal.)
RN 117-89-5 HCAPLUS
CN 10H-Phenothiazine, 10-[3-(4-methyl-1-piperazinyl)propyl]-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 6 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:306898 HCAPLUS
DOCUMENT NUMBER: 141:20324
TITLE: Ambler class A extended-spectrum beta-lactamase-producing Escherichia coli and Klebsiella spp. in Canadian hospitals
AUTHOR(S): Mulvey, Michael R.; Bryce, Elizabeth; Boyd, David; Ofner-Agostini, Marianna; Christianson, Sara; Simor, Andrew E.; Paton, Shirley
CORPORATE SOURCE: The Canadian Hospital Epidemiology Committee of The Canadian Nosocomial Infection Surveillance Program, Health Canada, Nosocomial Infections, National Microbiology Laboratory, Health Canada, Winnipeg, MB, Can.
SOURCE: Antimicrobial Agents and Chemotherapy (2004), 48(4), 1204-1214
CODEN: AMACCQ; ISSN: 0066-4804
PUBLISHER: American Society for Microbiology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB This report describes a study carried out to gain baseline information on the mol. characteristics of extended-spectrum beta-lactamase (ESBL)-producing Escherichia coli and Klebsiella spp. in Canada. A total of 29,323 E. coli and 5,156 Klebsiella sp. isolates were screened at 12 participating sites. Of these, 505 clin. significant, nonrepeat isolates displaying reduced susceptibility to the NCCLS-recommended beta-lactams were submitted to a central laboratory over a 1-yr period ending on 30 Sept. 2000. A total of 116 isolates were confirmed to be ESBL producers. PCR and sequence anal. revealed the presence of TEM-11 (n = 1), TEM-12 (n = 1), TEM-29 (n = 1), TEM-52 (n = 4), CTX-M-13 (n = 1), CTX-M-14 (n = **15**), CTX-M-15 (n = 11), SHV-2 (n = 2), SHV-2a (n = 12), SHV-5 (n = 6), SHV-12 (n = 45), and SHV-30 (n = 2). Five novel beta-lactamases were identified and designated TEM-115 (n = 2), TEM-120 (n = 1), SHV-40 (n = 2), SHV-41 (n = 4), and SHV-42 (n = 1). In addition, no mol. mechanism was identified for five isolates displaying an ESBL phenotype. Macrorestriction anal. of all ESBL isolates was conducted, as was restriction **fragment** length polymorphism anal. of plasmids harboring ESBLs. Although a "clonal" distribution of isolates was observed at some individual sites, there was very little evidence suggesting intrahospital spread. In addition, examples of identical or closely related

plasmids that were identified at geog. distinct sites across Canada are given. However, there was considerable diversity with respect to plasmid types observed

CC 10-5 (Microbial, Algal, and Fungal Biochemistry)
Section cross-reference(s): 14

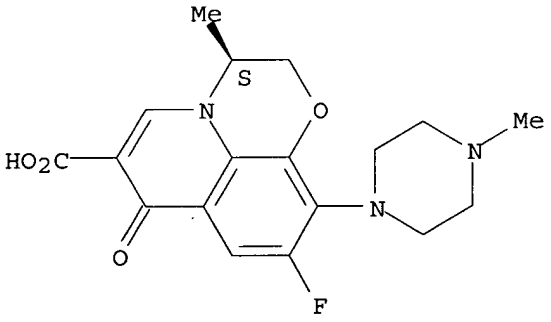
IT 67-20-9, Nitrofurantoin 69-53-4, Ampicillin 1403-66-3, Gentamicin 8064-90-2 25953-19-9, Cefazolin 32986-56-4, Tobramycin 35607-66-0, Cefoxitin 37517-28-5, Amikacin 63527-52-6, Cefotaxime 64221-86-9, Imipenem 69712-56-7, Cefotetan 72558-82-8, Ceftazidime 73384-59-5, Ceftriaxone 78110-38-0, Aztreonam 79198-29-1, Amoxicillin/clavulanic acid 80210-62-4, Cefpodoxime 85721-33-1, Ciprofloxacin 88040-23-7, Cefepime 96036-03-2, Meropenem **100986-85-4**, Levofloxacin 123683-33-0 123683-34-1 130005-95-7, Ceftazidime/clavulanic acid 130057-57-7, Cefotaxime/clavulanic acid 209742-13-2, Ceftriaxone/clavulanic acid 491877-29-3, Cefpodoxime/clavulanic acid
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(ambler class extended-spectrum beta-lactamase-producing Escherichia coli and Klebsiella spp. in Canadian hospitals)

IT **100986-85-4**, Levofloxacin
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(ambler class extended-spectrum beta-lactamase-producing Escherichia coli and Klebsiella spp. in Canadian hospitals)

RN 100986-85-4 HCAPLUS

CN 7H-Pyrido[1,2,3-de]-1,4-benzoxazine-6-carboxylic acid, 9-fluoro-2,3-dihydro-3-methyl-10-(4-methyl-1-piperazinyl)-7-oxo-, (3S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 7 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:633262 HCAPLUS
DOCUMENT NUMBER: 138:153509
TITLE: Synthesis of 8-chloro-11-(4-methyl-1-piperazinyl)-11-[14C]-dibenz[b,f][1,4]oxazepine
AUTHOR(S): Matloubi, Hojatollah; Ghandi, Mehdi; Saemian, Nader
CORPORATE SOURCE: Chem. Div., Nuclear Research Center/AEOI, Tehran, 11365-8486, Iran
SOURCE: Applied Radiation and Isotopes (2002), 57(4), 501-504
CODEN: ARISEF; ISSN: 0969-8043
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:153509
AB 8-Chloro-11-(4-methyl-1-piperazinyl)dibenz[b,f][1,4]oxazepine labeled with

carbon-14 in 11-position was prepared from 2-hydroxybenzonitrile-[cyano-14C].

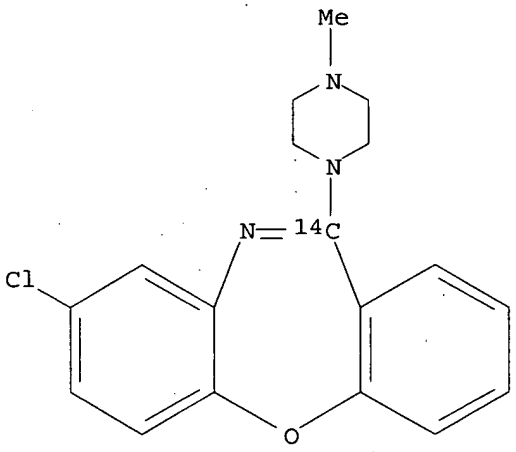
CC 28-22 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 8

IT **496839-47-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of carbon-14 labeled chloro(methylpiperazinyl)dibenz[b,f][1,4]oxazepine)

IT **496839-47-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of carbon-14 labeled chloro(methylpiperazinyl)dibenz[b,f][1,4]oxazepine)

RN 496839-47-5 HCAPLUS

CN Dibenz[b,f][1,4]oxazepine-11-14C, 8-chloro-11-(4-methyl-1-piperazinyl)-(9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 8 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:323121 HCAPLUS

DOCUMENT NUMBER: 137:185091

TITLE: A convenient synthesis of [11C]paraquat and other [N-methyl-11C]bisquaternary ammonium compounds

AUTHOR(S): Jewett, Douglas M.; Kilbourn, Michael R.

CORPORATE SOURCE: Division of Nuclear Medicine, Department of Radiology, University of Michigan Medical Center, Ann Arbor, MI, 48109-0552, USA

SOURCE: Journal of Labelled Compounds & Radiopharmaceuticals (2002), 45(4), 281-289
CODEN: JLCRD4; ISSN: 0362-4803

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

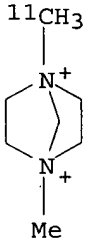
OTHER SOURCE(S): CASREACT 137:185091

AB [11C]Paraquat was synthesized by the reaction of [11C]methyl triflate with the mono-triflate salt of 1-methyl-[4,4']bipyridinyl. The product was selectively separated from the precursor by a microcolumn of Chelex 100 ion exchange resin. The method was applied to the synthesis of a variety of [N-methyl-11C]bisquaternary ammonium compds. This is the first reported use of a chelating cation exchange resin for the selective purification of organic

dications.
CC 21-2 (General Organic Chemistry)
Section cross-reference(s): 26
IT 452069-30-6P **452069-34-0P** 452069-37-3P 452069-40-8P
452069-43-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation [11C]paraquat and other [N-methyl-11C]bisquaternary ammonium compds.)
IT 67121-15-7P **452069-45-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation [11C]paraquat and other [N-methyl-11C]bisquaternary ammonium compds. and their isolation on chelating resin)
IT **452069-34-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation [11C]paraquat and other [N-methyl-11C]bisquaternary ammonium compds.)
RN 452069-34-0 HCAPLUS
CN 1,4-Diazoniabicyclo[2.2.1]heptane, 1-methyl-4-(methyl-11C)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

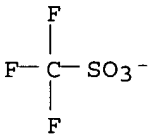
CM 1

CRN 452069-33-9
CMF C7 H16 N2



CM 2

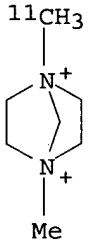
CRN 37181-39-8
CMF C F3 O3 S



IT **452069-45-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation [11C]paraquat and other [N-methyl-11C]bisquaternary ammonium compds. and their isolation on chelating resin)
RN 452069-45-3 HCAPLUS
CN 1,4-Diazoniabicyclo[2.2.1]heptane, 1-methyl-4-(methyl-11C)-, diiodide (9CI) (CA INDEX NAME)

CM 1

CRN 452069-33-9
CMF C7 H16 N2



CM 2

CRN 20461-54-5
CMF I

I^-

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 9 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:725193 HCAPLUS
DOCUMENT NUMBER: 139:32571
TITLE: Comparative distribution of binding of the muscarinic receptor ligands pirenzepine, AF-DX 384, (R,R)-I-QNB and (R,S)-I-QNB to human brain
AUTHOR(S): Piggott, Margaret; Owens, Jonathan; O'Brien, John; Paling, Sean; Wyper, David; Fenwick, John; Johnson, Mary; Perry, Robert; Perry, Elaine
CORPORATE SOURCE: Centre Development in Clinical Brain Ageing, MRC/University of Newcastle, Newcastle General Hospital, Newcastle-upon-Tyne, NE4 6BE, UK
SOURCE: Journal of Chemical Neuroanatomy (2002), 24(3), 211-223
CODEN: JCNAEE; ISSN: 0891-0618
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Quinuclidinyl benzilate (QNB) and its derivs. are being developed to investigate muscarinic receptor changes in vivo in Alzheimer's disease and dementia with Lewy bodies. This is the first study of [125I]-(R,R)-I-QNB and [125I]-(R,S)-I-QNB binding in vitro in human brain. We have compared the in vitro binding of the muscarinic ligands [3H]pirenzepine and [3H]AF-DX 384, which have selectivity for the M1 and M2/M4 receptor subtypes, resp., to the binding of [125I]-(R,R)-I-QNB and [125I]-(R,S)-I-QNB. This will provide a guide to the interpretation of in vivo SPET images generated with [123I]-(R,R)-I-QNB and [123I]-(R,S)-I-QNB. Binding was investigated in striatum, globus pallidus, thalamus and cerebellum, and cingulate, insula, temporal and occipital cortical areas, which show different proportions of muscarinic receptor subtypes, in post-mortem brain from normal individuals. M1 receptors are of high d. in

cortex and striatum and are relatively low in the thalamus and cerebellum, while M4 receptors are mainly expressed in the striatum, and M2 receptors are most evident in the cerebellum and thalamus. [125I]-(R,R)-I-QNB and [125I]-(R,S)-I-QNB d. distribution patterns were consistent with binding to both M1 and M4 receptors, with [125I]-(R,R)-I-QNB addnl. binding to a non-cholinergic site not displaceable by atropine. This distribution can be exploited by in vivo imaging, developing ligands for both SPET and PET, to reveal muscarinic receptor changes in Alzheimer's disease and dementia with Lewy bodies during the disease process and following cholinergic therapy.

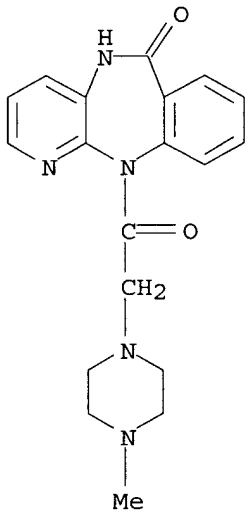
CC 8-9 (Radiation Biochemistry)

IT 88000-58-2 88000-63-9 **124620-97-9** 140186-38-5
RL: BSU (Biological study, unclassified); DGN (Diagnostic use); BIOL (Biological study); USES (Uses)
(comparative distribution of binding of the muscarinic receptor ligands pirenzepine, AF-DX 384, (R,R)-I-QNB and (R,S)-I-QNB to human brain)

IT **124620-97-9**
RL: BSU (Biological study, unclassified); DGN (Diagnostic use); BIOL (Biological study); USES (Uses)
(comparative distribution of binding of the muscarinic receptor ligands pirenzepine, AF-DX 384, (R,R)-I-QNB and (R,S)-I-QNB to human brain)

RN 124620-97-9 HCAPLUS

CN 6H-Pyrido[2,3-b][1,4]benzodiazepin-6-one, 5,11-dihydro-11-[(4-methyl-1-piperazinyl)acetyl]-, labeled with tritium (9CI) (CA INDEX NAME)



REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 10 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:802418 HCAPLUS

DOCUMENT NUMBER: 136:279425

TITLE: Modified synthesis of 11-[14C]-clozapine

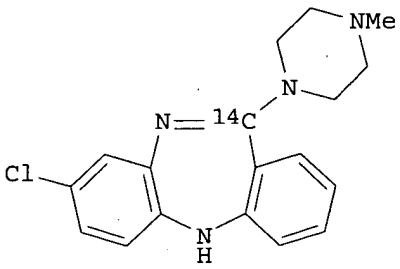
AUTHOR(S): Matloubi, Hojatollah; Ghandi, Mehdi; Zarrindast, Mohammad-Reza; Saemian, Nader

CORPORATE SOURCE: Nuclear Research Center/AEOI, Chemical Division, Tehran, Iran

SOURCE: Applied Radiation and Isotopes (2001), 55(6), 789-791
CODEN: ARISEF; ISSN: 0969-8043

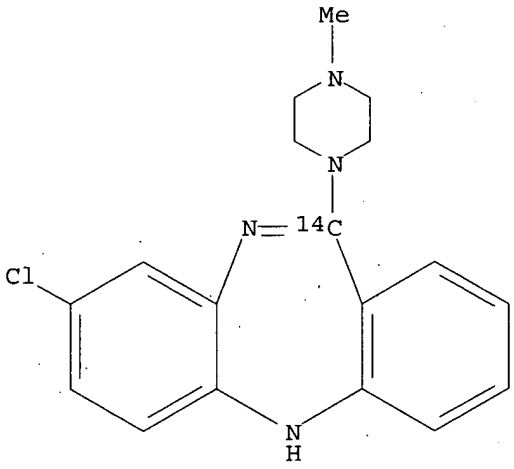
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:279425
GI



I

AB The reported synthetic pathway of the title compound (I) was modified in several steps. The synthetic pathway was shortened by 60%, and the total yield was increased from 6 to 23%.
CC 28-21 (Heterocyclic Compounds (More Than One Hetero Atom))
IT **146137-54-4**
RL: MSC (Miscellaneous)
(preparation of)
IT **146137-54-4**
RL: MSC (Miscellaneous)
(preparation of)
RN 146137-54-4 HCAPLUS
CN 5H-Dibenzo[b,e][1,4]diazepine-11-14C, 8-chloro-11-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 11 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:518471 HCAPLUS
DOCUMENT NUMBER: 136:273830
TITLE: Detection of quinolone resistance-determining regions

of gyrA gene of ofloxacin resistant chicken Escherichia coli

AUTHOR(S): Lei, Liancheng; Han, Wenyu; Wang, Xinglong; Wang, Shiruo; Feng, Xianwei; Jiang, Wenzheng; Chen, Wei

CORPORATE SOURCE: Faculty of Animal Science and Technology, Quartermaster University of PLA, Changchun, 130062, Peop. Rep. China

SOURCE: Zhongguo Shouyi Xuebao (2001), 21(3), 266-269
CODEN: ZSXUF5; ISSN: 1005-4545

PUBLISHER: Zhongguo Shouyi Xuebao Bianjibu

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB Thirteen ofloxacin-resistant strains of chicken pathogenic E.coli were from isolated clin. samples. After plasmid extraction and purification, the quinolone resistance-determining region (QRDR) of the gyrA gene was amplified by PCR with the plasmid templates. The plasmid PCR products were obtained from one strain, QRDR of the gyrA gene was also amplified by PCR from the templates of chromosomal DNA of this strain, then the PCR products were sequenced and analyzed. A expected 668-bp gyrA **fragments** was amplified from both plasmid DNA and chromosomal DNA of strain CE01. The nucleotide sequences of the PCR products of plasmid DNA and chromosomal DNA showed 98.17% homol. When compared to the corresponding sequences of gyrA of E. coli from the nucleotide sequence data reported by Swanberg S.L. and Wang J.**C.**, **13** mutant sites were found in the nucleotide sequence of PCR product from plasmid DNA, and 3 amino acids changed; while 12 mutant sites were found in that from chromosomal DNA, and 2 amino acids changed. The results showed that the quinolone resistant gene occurred both in the plasmid and chromosome of strain CE01 would be associated with quinolone resistance of strain CE01.

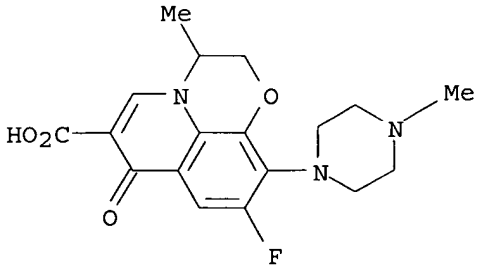
CC 3-3 (Biochemical Genetics)
Section cross-reference(s): 10

IT **82419-36-1**, Ofloxacin
RL: ARU (Analytical role, unclassified); ANST (Analytical study)
(chicken E. coli resistant to; detection of quinolone resistance-determining region of gyrA gene of ofloxacin resistant chicken Escherichia coli)

IT **82419-36-1**, Ofloxacin
RL: ARU (Analytical role, unclassified); ANST (Analytical study)
(chicken E. coli resistant to; detection of quinolone resistance-determining region of gyrA gene of ofloxacin resistant chicken Escherichia coli)

RN 82419-36-1 HCAPLUS

CN 7H-Pyrido[1,2,3-de]-1,4-benzoxazine-6-carboxylic acid, 9-fluoro-2,3-dihydro-3-methyl-10-(4-methyl-1-piperazinyl)-7-oxo- (9CI) (CA INDEX NAME)



L95 ANSWER 12 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:754931 HCAPLUS
DOCUMENT NUMBER: 132:151336
TITLE: Biologically active 11C-labeled amides using palladium-mediated reactions with aryl halides and [11C]carbon monoxide
AUTHOR(S): Kihlberg, Tor; Lngstroem, Bengt
CORPORATE SOURCE: Department of Organic Chemistry Institute of Chemistry and Uppsala University PET Centre, Uppsala University, Uppsala, S-751 85, Swed.
SOURCE: Journal of Organic Chemistry (1999), 64(25), 9201-9205
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:151336

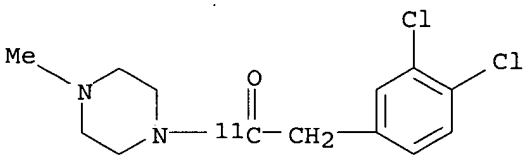
AB Using [11C]carbon monoxide in palladium-mediated synthesis, six amides were labeled with 11C. Ph and benzyl halides, e.g., 1,4-diiodobenzene and 3,4-dichlorobenzyl bromide, with halides as addnl. substituents were carbonylated and reacted with primary and secondary amines, e.g., N-methylpiperazine and 4-amino-N-benzylpiperidine. Four of the selected amides were receptor ligands, one was a precursor to a receptor ligand, and one was a model compound The 11C-labeled amides were obtained with good to almost quant. radiochem. yields with specific activities up to 1000 GBq/μmol. The radiochem. purity of the final products exceeded 98%. In one case, the corresponding 13C-substituted compound was produced to verify the position of the label. In a typical experiment starting with 5.0 GBq of [11C]carbon monoxide, 2.2 GBq of LC-purified N-(2-aminoethyl)-4-chloro[carbonyl-11C]benzamide was obtained within 15 min from the start of the carbonylation reaction (74% decay-corrected radiochem. yield). The presented approach gives significant new possibilities for 11C-labeling and is seen to be valuable also for synthesis of 13C- and 14C-substituted compds.

CC 21-2 (General Organic Chemistry)

IT **257862-19-4P** 257862-20-7P 257862-21-8P 257862-22-9P
257862-23-0P 257862-24-1P 257862-25-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of carbon-11 labeled amides via carbonylation of aryl halides and amines with carbon-11 labeled carbon monoxide)

IT **257862-19-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of carbon-11 labeled amides via carbonylation of aryl halides and amines with carbon-11 labeled carbon monoxide)

RN 257862-19-4 HCAPLUS
CN Piperazine, 1-[(3,4-dichlorophenyl)acetyl-1-11C]-4-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 13 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:738997 HCAPLUS

DOCUMENT NUMBER: 130:139034
TITLE: 13C CP (cross-polarization) MAS (magic angle spinning) NMR and GIAO-CHF calculations of buspirone analogs. Part 1. 3a,4,7,7a-Tetrahydro-2-[4-[4-(2-quinolinyl)-1-piperazinyl]butyl]-4,7-ethane-1H-isoindole-1,3(2H)-dione hydrochloride and hydrobromide
AUTHOR(S): Szelejewska-Wozniakowska, A.; Chilmonczyk, Z.; Les, A.; Wawer, I.
CORPORATE SOURCE: Pharmaceutical Research Institute, Warsaw, 01-793, Pol.
SOURCE: Solid State Nuclear Magnetic Resonance (1998), 13(1-2), 63-70
CODEN: SSNRE4; ISSN: 0926-2040
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 13C CP (cross-polarization) MAS (magic-angle spinning) solid-state NMR spectra of the title buspirone analogs were recorded. In the spectra of the hydrochloride and hydrobromide, 2 sets of signals appeared, in agreement with single-crystal x-ray-diffraction data indicating that 2 independent cations were present in the crystal unit in each salt. The largest shielding differences of 3.2-4.6 ppm between 2 sets of signals were found for quinoline aromatic C atoms C-3 and C-2. Ab initio calcns. of the C and N shielding consts. were performed by the GIAO-CHF method for structural **fragments**: N-butylsuccinimide, quinolinyl(N-methyl)piperazine-HCl and -HBr. Linear correlations between theor. and solid-state results were obtained, thus enabling a reasonable assignment of C resonances of the conformations present in the solid state. Due to the fast dynamics in solution, the C chemical shifts corresponded to the averaged values of the forms present in the solid state.

CC 22-10 (Physical Organic Chemistry)

IT GIAO (gauge invariant atomic orbital)
(CHF; **carbon-13** CP MAS NMR and GIAO-CHF calcns. of buspirone analog tetrahydro[[(quinolinyl)piperazinyl]butyl]ethanoisoindole hydrochloride and hydrobromide)

IT NMR (nuclear magnetic resonance)
(CP MAS; **carbon-13** CP MAS NMR and GIAO-CHF calcns. of buspirone analog tetrahydro[[(quinolinyl)piperazinyl]butyl]ethanoisoindole hydrochloride and hydrobromide)

IT Conformation
Crystal structure
Molecular structure
Nuclear shielding
(**carbon-13** CP MAS NMR and GIAO-CHF calcns. of buspirone analog tetrahydro[[(quinolinyl)piperazinyl]butyl]ethanoisoindole hydrochloride and hydrobromide)

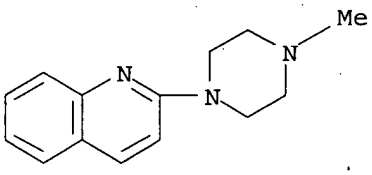
IT NMR (nuclear magnetic resonance)
(chemical shift; **carbon-13** CP MAS NMR and GIAO-CHF calcns. of buspirone analog tetrahydro[[(quinolinyl)piperazinyl]butyl]ethanoisoindole hydrochloride and hydrobromide)

IT 3470-96-0, N-Butylsuccinimide 36505-84-7D, Buspirone, analogs
50398-09-9, N-Methylpiperazine hydrochloride 195194-85-5 195194-87-7
220073-79-0 220073-80-3
RL: PRP (Properties)
(**carbon-13** CP MAS NMR and GIAO-CHF calcns. of buspirone analog tetrahydro[[(quinolinyl)piperazinyl]butyl]ethanoisoindole hydrochloride and hydrobromide)

IT **220073-79-0 220073-80-3**
RL: PRP (Properties)
(**carbon-13** CP MAS NMR and GIAO-CHF calcns. of

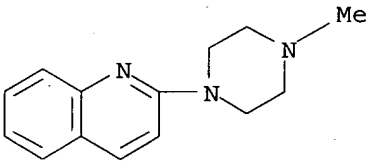
buspirone analog tetrahydro[[(quinolinyl)piperazinyl]butyl]ethanoisoindole hydrochloride and hydrobromide)

RN 220073-79-0 HCAPLUS
CN Quinoline, 2-(4-methyl-1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 220073-80-3 HCAPLUS
CN Quinoline, 2-(4-methyl-1-piperazinyl)-, monohydrobromide (9CI) (CA INDEX NAME)



● HBr

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 14 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:622009 HCAPLUS
DOCUMENT NUMBER: 127:259504
TITLE: Synthesis and biodistribution of two potential PET radioligands for dopamine reuptake sites: no-carrier-added 4-(2-[18F]fluoroethyl) and 4-[11C]methyl BTCP-piperazine
AUTHOR(S): Loustau-Then, I.; Ponchant, M.; Fuseau, C.; Kamenka, J. M.; Vignon, J.; Crouzel, C.
CORPORATE SOURCE: D.R.M., SERVICE HOSPITALIER FREDERIC-JOLIOT, CEA, ORSAY, 91406, Fr.
SOURCE: Nuclear Medicine and Biology (1997), 24(6), 513-518
CODEN: NMBIEO; ISSN: 0969-8051
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Radioligands that specifically target dopamine uptake sites can provide a means of determining dopamine fiber loss at intrastriatal mesencephalic grafts in Parkinsonian patients, using Positron Emission Tomog. (PET). The BTCP derivative, 1-[1-(2-benzo(b)thiophenyl)cyclohexyl]-4-(2-hydroxyethyl)-piperazine, shows in vitro high affinity and selectivity for the dopamine

transporter. To evaluate the potential of such a compound as a potential dopaminergic PET tracer the positron-emitting analogs, 1-[1-(2-benzo(b)thiophenyl)cyclohexyl]-4-(2-[18F]fluoroethyl)-piperazine and 1-[1-(2-benzo(b)thiophenyl)cyclohexyl]-4-[11C]methylpiperazine, were synthesized. Radiofluorination was carried out by the reaction of 1-[1-(2-benzo(b)thiophenyl)cyclohexyl]-4-(2-chloroethyl)-piperazine with cyclotron-produced n.c.a. 18F-(half life 109.9 min) obtained by the (p,n) reaction on 18O-enriched water. Labeling with carbon-11 (half life 20.4 min) was achieved by 11C methylation of 1-[1-(2-benzo(b)thiophenyl)cyclohexyl]-piperazine with [11C]methyl iodide. After i.v. administration to rats these two compds. enter the brain, but despite their high in vitro affinity they display a high non specific binding in vivo which greatly limits their use as PET radioligands.

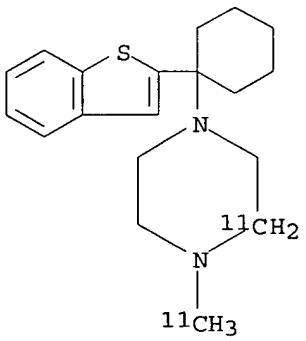
CC 8-9 (Radiation Biochemistry)

IT 176910-95-5P **196093-78-4P**
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(synthesis and biodistribution of two potential PET radioligands for dopamine reuptake sites: 4-(2-[18F]fluoroethyl) and 4-[11C]methyl-BTCP-piperazine)

IT **196093-78-4P**
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(synthesis and biodistribution of two potential PET radioligands for dopamine reuptake sites: 4-(2-[18F]fluoroethyl) and 4-[11C]methyl-BTCP-piperazine)

RN 196093-78-4 HCAPLUS

CN Piperazine-2-11C, 4-(1-benzo[b]thien-2-ylcyclohexyl)-1-(methyl-11C)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 15 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:738115 HCAPLUS

DOCUMENT NUMBER: 128:43944

TITLE: Use of [3H]-clozapine as a ligand of the dopamine D4 receptor subtype in peripheral tissues

AUTHOR(S): Ricci, A.; Bronzetti, E.; Rossodivita, I.; Amenta, F.

CORPORATE SOURCE: Sezione di Anatomia Umana, Dipartimento di Scienze Farmacologiche e Medicina Sperimentale, Universita di Camerino, Camerino, 62032, Italy

SOURCE: Journal of Autonomic Pharmacology (1997), 17(4),

261-267
CODEN: JAPHDU; ISSN: 0144-1795
PUBLISHER: Blackwell Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

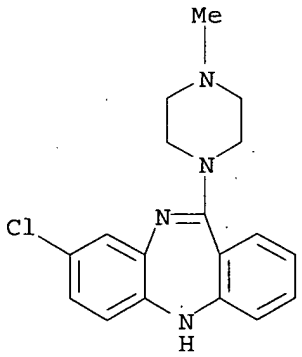
AB Mol. biol. studies have documented the presence of peripheral dopamine D4 receptors. This site has not been characterized yet with classical radioligand binding assay techniques because of the lack of selective radioligands. The atypical neuroleptic clozapine labeled with tritium ([3H]-clozapine) has been proposed and sold as a radioligand for brain dopamine D4 receptors. However, the selectivity of [3H]-clozapine for D4 receptor subtypes, and its specificity for brain dopamine receptors, have been questioned. In this study dopamine D4 receptors were assayed in peripheral organs known to express them, such as rat atria and kidney, by using a radioligand binding assay technique with [3H]-clozapine as the radioligand. Parallel expts. were performed using Chinese hamster ovary (CHO) cells transfected with the D4 receptor clone (variant D4.2). [3H]-Clozapine was bound to sections of rat atria and kidney. After appropriate blockade of sites other than dopamine receptors to which it can bind (i.e. muscarinic cholinergic, serotonergic and α-adrenergic receptors), the radioligand was bound to a site displaying a pharmacol. profile similar to that expressed by CHO cells transfected with the D4 receptor. The above findings indicate that with appropriate protocols, [3H]-clozapine may represent a radioligand for peripheral dopamine D4 receptors.

CC 2-1 (Mammalian Hormones)
Section cross-reference(s): 8

IT **119550-28-6**
RL: BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); PROC (Process); USES (Uses)
(use of [3H]-clozapine as a ligand of dopamine D4 receptor subtype in peripheral tissues)

IT **119550-28-6**
RL: BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); PROC (Process); USES (Uses)
(use of [3H]-clozapine as a ligand of dopamine D4 receptor subtype in peripheral tissues)

RN 119550-28-6 HCAPLUS
CN 5H-Dibenzo[b,e][1,4]diazepine, 8-chloro-11-(4-methyl-1-piperazinyl)-, labeled with tritium (9CI) (CA INDEX NAME)



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 16 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:954807 HCAPLUS
DOCUMENT NUMBER: 123:329971
TITLE: Enhancement of the efficacy of drugs by deuteration
INVENTOR(S): Foster, Robert R.; Lewanczuk, Richard; Caille, Gilles
PATENT ASSIGNEE(S): Isotechnika Inc., Can.
SOURCE: PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

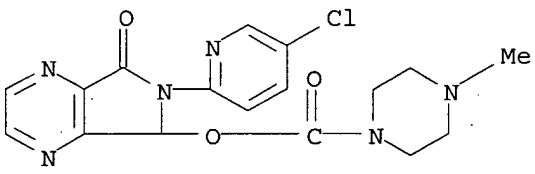
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9526325	A2	19951005	WO 1995-CA154	19950327
WO 9526325	A3	19951214		
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, UZ				
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2186371	AA	19951005	CA 1995-2186371	19950327
AU 9519441	A1	19951017	AU 1995-19441	19950327
AU 707748	B2	19990722		
EP 751926	A1	19970108	EP 1995-912109	19950327
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
CN 1148843	A	19970430	CN 1995-193186	19950327
CN 1087725	B	20020717		
BR 9507200	A	19970916	BR 1995-7200	19950327
JP 09510717	T2	19971028	JP 1995-524885	19950327
JP 3696884	B2	20050921		
AU 9944783	A1	20000224	AU 1999-44783	19990827
AU 747744	B2	20020523		

PRIORITY APPLN. INFO.: US 1994-217897 A 19940325
WO 1995-CA154 W 19950327

AB A method of enhancing the efficiency and increasing the duration of action of drugs (e.g. dihydropyridines) and particularly of nifedipine is described, wherein ≥1 H atoms are replaced by D and wherein the deuterated nifedipine has unexpectedly improved hypotensive properties when used in much lower concns. than nifedipine per se. A method for determining the identity and bioequivalency of a new drug is also disclosed, wherein the mol. and **isotope** structure of a new drug is determined by gas chromatog.-**isotope** ratio mass spectrometry and compared with the mol. and **isotope** structure of a known human drug. Thus, nifedipine was 95% deuterated on the C-2 and C-6 Me groups by incubation with (CD3)2CO and (F3CCO)2O in CDCl3-D2O. Nifedipine-d6 decreased the blood pressure of normotensive and spontaneously hypertensive rats more than did nondeuterated nifedipine, and showed greater use-dependent inhibition of Ca2+ channels in NIE-115 neuroblastoma cells.

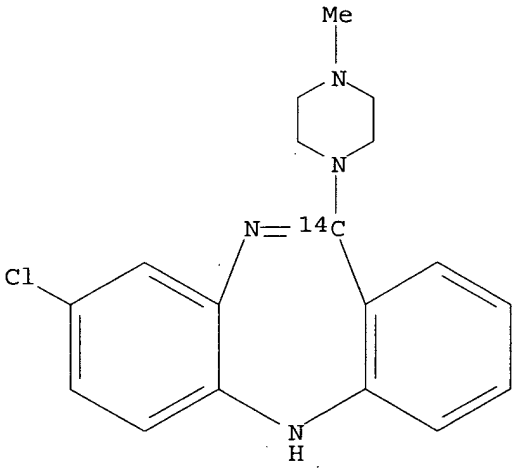
IC ICM C07B059-00
CC 1-3 (Pharmacology)
Section cross-reference(s): 64
IT Antihypertensives
Deuteration
Isotope effect

(enhancement of efficacy of drugs by deuteration)
IT Hair
(**isotope** composition of, identification in relation to)
IT Alcoholic beverages
(**isotope** composition of, origin in relation to)
IT Chromatography, gas
(**isotope**-ratio mass spectrometry combined with, in pharmaceutical anal.; enhancement of efficacy of drugs by deuteration)
IT Mass spectrometry
(**isotope**-ratio, gas chromatog. combined with, in pharmaceutical anal.; enhancement of efficacy of drugs by deuteration)
IT Pharmaceutical analysis
(**isotopic**; enhancement of efficacy of drugs by deuteration)
IT 22071-15-4, Ketoprofen 37517-30-9, Acebutolol **43200-80-2**, Zopiclone 85721-33-1, Ciprofloxacin
RL: ANT (Analyte); ANST (Analytical study)
(**carbon-13** content of, origin in relation to)
IT 3337-17-5D, 1,4-Dihydropyridine, derivs., **isotopically** substituted 7440-44-0D, Carbon, **isotopes**, biological studies 7727-37-9D, Nitrogen, **isotopes**, biological studies 7782-44-7D, Oxygen, **isotopes**, biological studies 21829-25-4D, Nifedipine, **isotopically labeled** 22609-73-0D, Niludipine, **isotopically labeled** 39562-70-4D, Nitrendipine, **isotopically labeled** 55985-32-5D, Nicardipine, **isotopically labeled** 63675-72-9D, Nisoldipine, **isotopically labeled** 66085-59-4D, Nimodipine, **isotopically labeled** 72509-76-3D, Felodipine, **isotopically labeled** 75695-93-1D, Isradipine, **isotopically labeled** 88150-42-9D, Amlodipine, **isotopically labeled**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(enhancement of efficacy of drugs by deuteration)
IT 3930-20-9, Sotalol
RL: ANT (Analyte); ANST (Analytical study)
(**isotope** composition of, origin in relation to)
IT 14390-96-6, **Nitrogen-15**, analysis 14762-74-4, **Carbon-13**, analysis 14797-71-8, Oxygen-18, analysis
RL: ANT (Analyte); ANST (Analytical study)
(pharmaceutical origin in relation to content of)
IT **43200-80-2**, Zopiclone
RL: ANT (Analyte); ANST (Analytical study)
(**carbon-13** content of, origin in relation to)
RN 43200-80-2 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-methyl-, 6-(5-chloro-2-pyridinyl)-6,7-dihydro-7-oxo-5H-pyrrolo[3,4-b]pyrazin-5-yl ester (9CI) (CA INDEX NAME)



L95 ANSWER 17 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:101917 HCAPLUS

DOCUMENT NUMBER: 118:101917
TITLE: Synthesis of carbon-14 and tritium labeled analogs of the novel antischizophrenic agent clozapine
AUTHOR(S): Sunay, Ustun B.; Talbot, Kenrick C.; Galullo, Vincent
CORPORATE SOURCE: Isot. Lab., Sandoz Res. Inst., East Hanover, NJ, 07936, USA
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1992), 31(12), 1041-7
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Clozapine labeled with carbon-14 in the 11-position was prepared from 2-aminobenzonitrile-[cyano-14C]. In addition, clozapine was also labeled with C3H3 in the Me group of the 4-methylpiperazine ring.
CC 28-21 (Heterocyclic Compounds (More Than One Hetero Atom))
IT **146137-54-4P** 146137-55-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **146137-54-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 146137-54-4 HCAPLUS
CN 5H-Dibenzo[b,e][1,4]diazepine-11-14C, 8-chloro-11-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



L95 ANSWER 18 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:102104 HCAPLUS
DOCUMENT NUMBER: 116:102104
TITLE: Recent trends in receptor analysis techniques and instrumentation
AUTHOR(S): Palacios, J. M.; Mengod, G.; Vilaro, M. T.; Ramm, P.
CORPORATE SOURCE: Sandoz Pharma Ltd., Basel, 4002, Switz.
SOURCE: Journal of Chemical Neuroanatomy (1991), 4(5), 343-53
CODEN: JCNAEE; ISSN: 0891-0618
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Receptor autoradiog. allows visualization of receptor binding sites at the regional or light microscopic level. Receptor autoradiog. is a mature methodol., in widespread use. It is also a dynamic and expanding

methodol., benefiting constantly from the introduction of new techniques and instrumentation. In particular, receptor autoradiog. has taken advantage of image anal. instrumentation to provide efficient spatial mapping of receptor populations and their pharmacol. characteristics. A major contribution to the understanding of receptors has come from the recent cloning of the genes coding for many of these receptors. This has allowed the use of in situ hybridization to demonstrate the cells expressing mRNA coding for specific receptor subtypes. The result is that many receptor populations, previously thought to be homogeneous, are shown to be composed of several subtypes. As a consequence, the distribution of many receptors requires re-examination, which is aided by the development of new and more selective ligands. With the incorporation of techniques from mol. biol. into receptor autoradiog., the demands upon image anal. instruments have expanded. Over the past decade, densitometric image anal. have attained a high level of sophistication for classical receptor autoradiog. However, to serve the needs of today's receptor laboratory, an image analyzer must be equally capable in regional densitometry, in counting and spatial mapping of grain and or cell locations at the microscopic level, and in analyzing electrophoresis gels. Advances in image anal. hardware and software are keeping pace with the requirements of receptor labs. As an example, the authors illustrated here some of their results with muscarinic receptors.

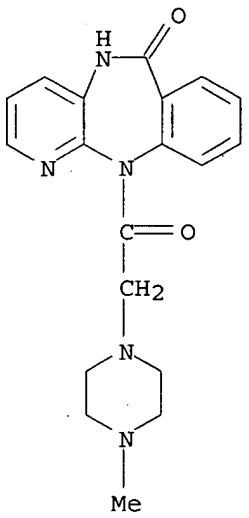
CC 9-8 (Biochemical Methods)

IT 83945-36-2 **124620-97-9** 131042-02-9 139182-85-7 140186-38-5
RL: ANST (Analytical study)
(autoradiog. with, of muscarinic receptors in brain, image anal. requirements for)

IT **124620-97-9**
RL: ANST (Analytical study)
(autoradiog. with, of muscarinic receptors in brain, image anal. requirements for)

RN 124620-97-9 HCAPLUS

CN 6H-Pyrido[2,3-b][1,4]benzodiazepin-6-one, 5,11-dihydro-11-[(4-methyl-1-piperazinyl)acetyl]-, labeled with tritium (9CI) (CA INDEX NAME)



L95 ANSWER 19 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:551512 HCAPLUS
DOCUMENT NUMBER: 113:151512

TITLE: Tritium labeling of simple 7-membered ring compounds
AUTHOR(S): Hiltunen, J.; Peng, C. T.; Yang, Z. C.
CORPORATE SOURCE: Sch. Pharm., Univ. California, San Francisco, CA, 94143-0446, USA
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1990), 28(5), 543-54
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English

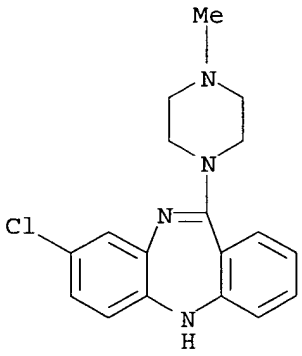
AB Seven-membered ring compds., from cycloheptane to complex ring structures containing heteroatoms, substituents and fused phenyl rings, were labeled with tritium, using activated and adsorbed tritium. The 7-membered ring structures are generally stable towards reactions with tritium, which allows compds. like 1-benzosuberone, 1-aza-2-methoxy-1-cycloheptene, iminostilbene and clozapine to be labeled to reasonably high specific activities. The best method varies greatly from compound to compound By optimizing the labeling conditions and use of efficient support exceptionally good results can be obtained. Of several adsorbents studied, the Pd-on-alumina support gives consistently products of the highest specific activity with least radioimpurity. Even mols. containing carbon-halogen bond and hydrogen bound to nitrogen can usually be labeled with tritium at stable positions and without dehalogenation.

CC 21-2 (General Organic Chemistry)
Section cross-reference(s): 63, 71

IT 62696-10-0P **119550-28-6P** 129549-74-2P 129549-76-4P
129549-79-7P 129549-81-1P 129549-82-2P, preparation 129549-83-3P
129549-84-4P, Azulene-1,3-t2 129549-85-5P 129549-86-6P 129549-87-7P
129549-88-8P 129549-89-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and specific activity determination of)

IT **119550-28-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and specific activity determination of)

RN 119550-28-6 HCAPLUS
CN 5H-Dibenzo[b,e][1,4]diazepine, 8-chloro-11-(4-methyl-1-piperazinyl)-, labeled with tritium (9CI) (CA INDEX NAME)



L95 ANSWER 20 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:452079 HCAPLUS
DOCUMENT NUMBER: 113:52079
TITLE: Telenzepine enantiomers block muscarinic M1-receptors with opposite kinetics
AUTHOR(S): Eltze, Manfrid

CORPORATE SOURCE: Dep. Pharmacol., Byk Gulden Pharm., Konstanz, D-7750, Germany
SOURCE: European Journal of Pharmacology (1990), 180(1), 161-8
CODEN: EJPHAZ; ISSN: 0014-2999
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Stimulation of muscarinic M1-receptors in isolated rabbit vas deferens by McN-A-343 inhibited elec. induced twitch contractions, an effect which was competitively antagonized by (+)-, (±)-, and (-)-telenzepine and pirenzepine (pA2 = 9.12, 8.86, 6.98, and 7.79, resp.). The inhibition of twitch contractions by 10-6M McN-A-343 was reversed by the antimuscarinic agents (at concns. 10-fold higher than pA2) in a time-dependent manner. The antagonists were then displaced by 3 + 10-5M McN-A-343, which again led to inhibition of twitch contractions. Assuming 1st-order kinetics for M1-receptor blockade by the antagonists, half-time values for the start and end of blockade were calculated For (+)-telenzepine, the values for the rates for the start and end of blockade were 23 and 174 min, resp., whereas (-)-telenzepine exhibited an inverse kinetic pattern of 3.0 and 0.38 min, resp. The extremely slow dissociation of (+)-telenzepine from muscarinic M1-receptors may explain the long-lasting pharmacol. effect of this compound in vivo.

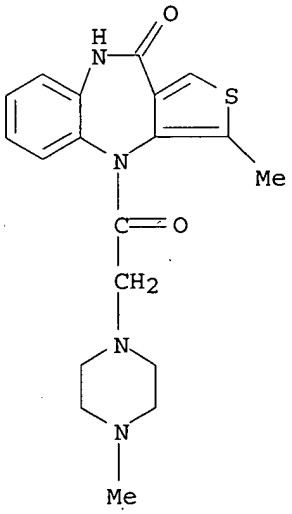
CC 1-3 (Pharmacology)

IT 28797-61-7, Pirenzepine **122195-38-4 122195-39-5 122219-70-9**
RL: BIOL (Biological study)
(muscarinic M1 receptors blockade by, kinetics of, stereoisomerism in relation to)

IT **122195-38-4 122195-39-5 122219-70-9**
RL: BIOL (Biological study)
(muscarinic M1 receptors blockade by, kinetics of, stereoisomerism in relation to)

RN 122195-38-4 HCAPLUS

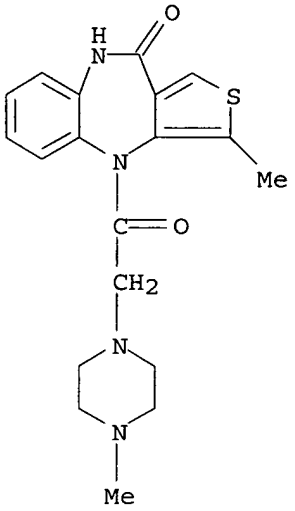
CN 10H-Thieno[3,4-b][1,5]benzodiazepin-10-one, 4,9-dihydro-3-methyl-4-[(4-methyl-1-piperazinyl)acetyl]-, labeled with tritium, (+)- (9CI) (CA INDEX NAME)



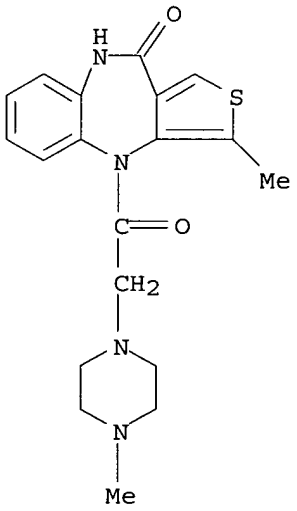
RN 122195-39-5 HCAPLUS

CN 10H-Thieno[3,4-b][1,5]benzodiazepin-10-one, 4,9-dihydro-3-methyl-4-[(4-methyl-1-piperazinyl)acetyl]-, labeled with tritium, (-)- (9CI) (CA INDEX

NAME)



RN 122219-70-9 HCAPLUS
CN 10H-Thieno[3,4-b][1,5]benzodiazepin-10-one, 4,9-dihydro-3-methyl-4-[(4-methyl-1-piperazinyl)acetyl]-, labeled with tritium (9CI) (CA INDEX NAME)



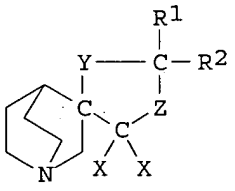
L95 ANSWER 21 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:48812 HCAPLUS
DOCUMENT NUMBER: 112:48812
TITLE: Novel oxathiolane derivatives their preparation, and their therapeutic use
INVENTOR(S): Fisher, Abraham; Karton, Ishai
PATENT ASSIGNEE(S): Israel Institute for Biological Research, Israel
SOURCE: Eur. Pat. Appl., 20 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 314444	A2	19890503	EP 1988-310040	19881026
EP 314444	A3	19901107		
EP 314444	B1	19960529		
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, LU, NL, SE				
US 4876260	A	19891024	US 1988-189210	19880502
IL 87834	A1	19920525	IL 1988-87834	19880922
ZA 8807326	A	19891129	ZA 1988-7326	19880929
AU 8823671	A1	19890504	AU 1988-23671	19881012
AU 608903	B2	19910418		
AT 138663	E	19960615	AT 1988-310040	19881026
ES 2087854	T3	19960801	ES 1988-310040	19881026
DK 8805986	A	19890429	DK 1988-5986	19881027
DK 175064	B1	20040517		
NO 8804790	A	19890502	NO 1988-4790	19881027
NO 167806	B	19910902		
NO 167806	C	19911211		
CA 1315791	A1	19930406	CA 1988-581526	19881027
JP 02062883	A2	19900302	JP 1988-271085	19881028
JP 2753280	B2	19980518		
IN 170689	A	19920502	IN 1990-MA426	19900530
IN 170320	A	19920314	IN 1990-MA455	19900611

PRIORITY APPLN. INFO.: US 1987-114473 A 19871028
US 1988-189210 A 19880502
IN 1988-MA695 A 19881005

OTHER SOURCE(S): CASREACT 112:48812; MARPAT 112:48812
GI

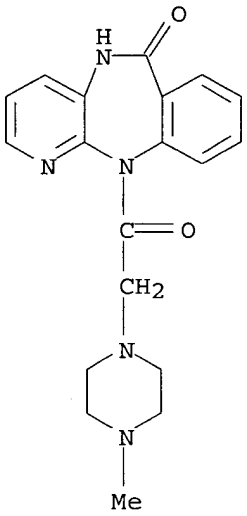


I

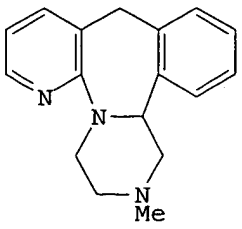
AB Spiro-oxathiolane/quinuclidine derivs. I [1 of Y and Z = O and the other is S(O)n (n = 0-2); R1, R2 = H, alkyl, alkenyl, etc. (at least R1 or R2 ≠ H); X = H (or when Y = O and Z = S(O)n simultaneously, X = 2H, 3H), etc.] and their geometric isomers, enantiomers, diastereomers, racemates, and acid addition salts, and pharmaceutical compns. containing them, are provided. I are useful as medicaments or diagnostic agents, or in the manufacture of medicaments and diagnostic agents, applicable to diseases or disorders of the central nervous or cholinergic system. Ten derivs. were tested for their ability, as compared with oxotremorine (mainly an M2 muscarinic receptor agonist) and McN-A-343 (mainly an M1 muscarinic receptor agonist), to displace tritiated quinuclidinyl benzilate (3H-QNB) from rat brain homogenates. The (-)-cis-2-methylspiro(1,3-oxathiolan-5,3')quinulcidine was 2.2 times more potent in 3H-QNB displacement than its racemate. Moreover, the latter was the most selective M1 agonist, being more selective than the prototype M1 agonist McN-A-343.

IC ICM C07D497-20
ICS C07B059-00; A61K031-435; A61K043-00

ICI C07D497-20, C07D327-00, C07D221-00
CC 1-11 (Pharmacology)
Section cross-reference(s): 28
IT 70761-70-5 **124620-97-9** 124620-98-0
RL: BIOL (Biological study)
(displacement from rat brain homogenate of, by spiro-oxathiolane/quinuclidine derivs.)
IT **124620-97-9**
RL: BIOL (Biological study)
(displacement from rat brain homogenate of, by spiro-oxathiolane/quinuclidine derivs.)
RN 124620-97-9 HCAPLUS
CN 6H-Pyrido[2,3-b][1,4]benzodiazepin-6-one, 5,11-dihydro-11-[(4-methyl-1-piperazinyl)acetyl]-, labeled with tritium (9CI) (CA INDEX NAME)



L95 ANSWER 22 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:139001 HCAPLUS
DOCUMENT NUMBER: 112:139001
TITLE: The synthesis of Org 3770 **labeled** with tritium, **carbon-13** and carbon-14
AUTHOR(S): Kaspersen, Frans M.; Van Rooij, Fons A. M.; Sperling, Eric G. M.; Wieringa, Joop H.
CORPORATE SOURCE: Sci. Dev. Group, Organon Int. BV, Oss, 5340 BH, Neth.
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1989), 27(9), 1055-68
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:139001
GI



I

AB The syntheses of 1,2,3,4,10,14b-hexahydro-2-methylpyrazino[2,1-a]pyrido[2,3-c][2]benzazepine (Org 3770, I) **labeled** with 3H (and 2H), 13C and 14C are described. Tritiated I was prepared either by exchange under alkaline conditions with tritiated water or catalytic reductive dehalogenation of a chloro analog with 3H2. 13C-**labeled** material was obtained in a 7-step synthesis starting from 13C-**labeled** benzene, whereas I-14C was prepared in a 3-step synthesis starting with 14CO2.

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

ST **isotopic labeling** Org 3770; pyrazinopyridobenzazepine hexahydromethyl **isotopic labeling**

IT **125967-24-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and carboxylation of)

IT 125770-91-4P **125770-92-5P** **125967-26-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)

IT **125967-23-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and diazotization-bromination of)

IT **125967-22-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenation of)

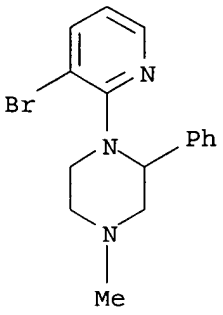
IT 125967-17-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with **labeled** bromoacetophenone)

IT 125967-20-6P 125967-21-7P **125967-25-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

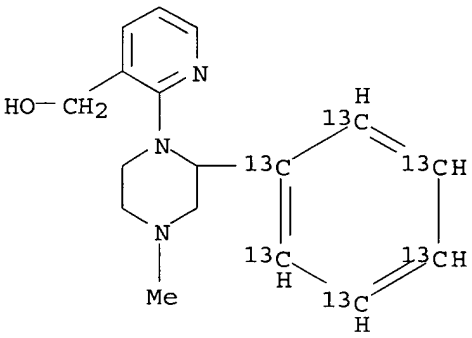
IT **125967-24-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and carboxylation of)

RN 125967-24-0 HCAPLUS

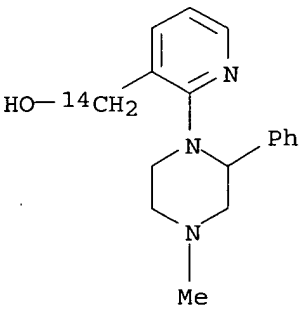
CN Piperazine, 1-(3-bromo-2-pyridinyl)-4-methyl-2-phenyl- (9CI) (CA INDEX NAME)



IT **125770-92-5P 125967-26-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)
RN 125770-92-5 HCAPLUS
CN 3-Pyridinemethanol, 2-[4-methyl-2-(phenyl-13C6)-1-piperazinyl]- (9CI) (CA INDEX NAME)

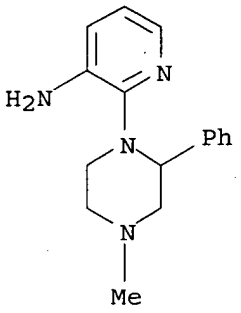


RN 125967-26-2 HCAPLUS
CN 3-Pyridinemethanol-α-14C, 2-(4-methyl-2-phenyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

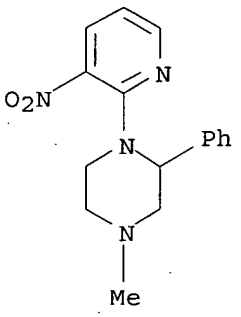


IT **125967-23-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and diazotization-bromination of)
RN 125967-23-9 HCAPLUS

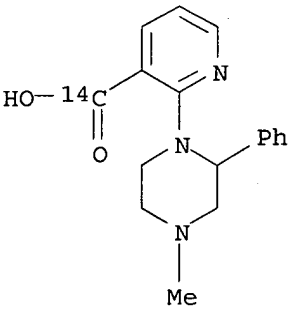
CN 3-Pyridinamine, 2-(4-methyl-2-phenyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



IT **125967-22-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenation of)
RN 125967-22-8 HCAPLUS
CN Piperazine, 4-methyl-1-(3-nitro-2-pyridinyl)-2-phenyl- (9CI) (CA INDEX NAME)



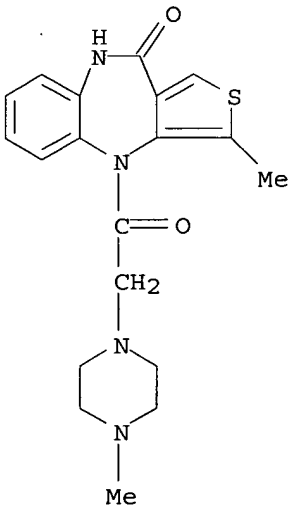
IT **125967-25-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 125967-25-1 HCAPLUS
CN 3-Pyridinecarboxylic-14C acid, 2-(4-methyl-2-phenyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



L95 ANSWER 23 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:151426 HCAPLUS
DOCUMENT NUMBER: 112:151426
TITLE: Cyproheptadine displays high affinity for muscarinic receptors but does not discriminate between receptor subtypes
AUTHOR(S): Eltze, Manfrid; Lambrecht, Guenter; Mutschler, Ernst
CORPORATE SOURCE: Dep. Pharmacol., Byk Gulden Pharm., Konstanz, D-7750, Fed. Rep. Ger.
SOURCE: European Journal of Pharmacology (1989), 173(2-3), 219-22
CODEN: EJPHAZ; ISSN: 0014-2999
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The affinity of cyproheptadine for different muscarinic receptor subtypes was investigated in vitro by functional expts. in field-stimulated vas deferens of the rabbit (ganglionic M1- and cardiac M2-receptors) and in guinea pig ileum (smooth muscle M3-receptors). Cyproheptadine displayed high but similar affinity for all muscarinic receptor subtypes studied (pA2 = 7.99-8.02). In contrast, (+)-telenzepine (M1 over M2 and M3) and mefurtramine (M2 over M3 and M1) were selective.

CC 1-7 (Pharmacology)
IT **122195-38-4** 126116-01-6
RL: BIOL (Biological study)
(muscarinic receptor subtypes response to, specificity of, cyproheptadine in relation to)
IT **122195-38-4**
RL: BIOL (Biological study)
(muscarinic receptor subtypes response to, specificity of, cyproheptadine in relation to).
RN 122195-38-4 HCAPLUS
CN 10H-Thieno[3,4-b][1,5]benzodiazepin-10-one, 4,9-dihydro-3-methyl-4-[(4-methyl-1-piperazinyl)acetyl]-, labeled with tritium, (+)- (9CI) (CA INDEX NAME)

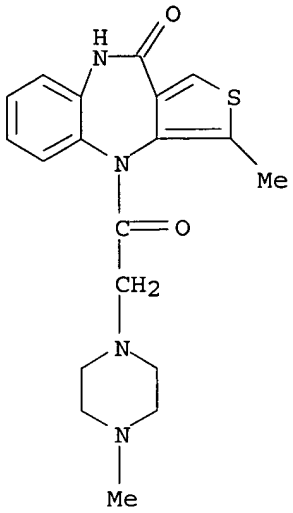


L95 ANSWER 24 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

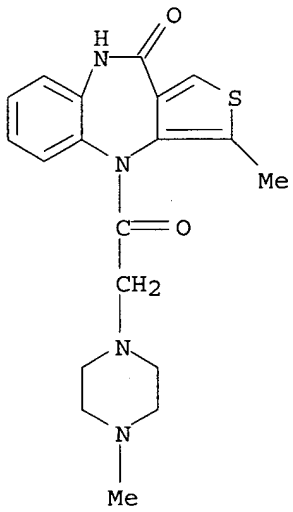
ACCESSION NUMBER: 1989:490172 HCAPLUS
DOCUMENT NUMBER: 111:90172
TITLE: The affinity, selectivity and biological activity of telenzepine enantiomers
AUTHOR(S): Schudt, C.; Boer, R.; Eltze, M.; Riedel, R.; Grundler, G.; Birdsall, N. J. M.
CORPORATE SOURCE: Dep. Pharmacol., Byk Gulden Res. Lab., Konstanz, D-7750, Fed. Rep. Ger.
SOURCE: European Journal of Pharmacology (1989), 165(1), 87-96
CODEN: EJPHAZ; ISSN: 0014-2999
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The binding of the enantiomers of telenzepine, an antiulcer drug, to muscarinic receptor subtypes in the guinea-pig cerebral cortex, myocardium and salivary glands was examined The (+)-enantiomer was more potent in all assays and exhibited a greater selectivity than the (-)-enantiomer for the different receptor subtypes in membrane prepns.. The enantiomeric potency ratio varied from .simeq.400 (cortical M1 receptors) to .simeq.50 (cardiac receptors). In functional assays in vitro in the rabbit vas deferens and rat atria, the affinity consts. and enantiomeric potency ratios for the 2 isomers agreed with those found in the binding assays. A high enantiomeric potency ratio, 180, was found in vivo for the ability of the telenzepine enantiomers to inhibit the production of stomach mucosal lesions in the modified Shay rat preparation The data are compatible with the blockade of M1 receptors by (+)-telenzepine and oppose the possibility that the anti-ulcer action of telenzepine is mediated via a muscarinic or non-muscarinic action of the (-)-enantiomer.

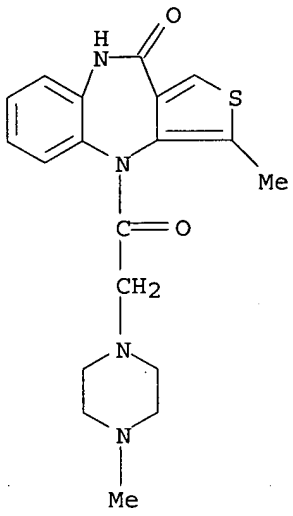
CC 1-9 (Pharmacology)
IT **122195-38-4 122195-39-5 122219-70-9**
RL: BIOL (Biological study)
(muscarinic receptor-blocking activity of, in ulcer inhibition, stereochem. in)
IT **122195-38-4 122195-39-5 122219-70-9**
RL: BIOL (Biological study)
(muscarinic receptor-blocking activity of, in ulcer inhibition, stereochem. in)
RN 122195-38-4 HCAPLUS
CN 10H-Thieno[3,4-b][1,5]benzodiazepin-10-one, 4,9-dihydro-3-methyl-4-[(4-methyl-1-piperazinyl)acetyl]-, labeled with tritium, (+)- (9CI) (CA INDEX NAME)



RN 122195-39-5 HCAPLUS
CN 10H-Thieno[3,4-b][1,5]benzodiazepin-10-one, 4,9-dihydro-3-methyl-4-[(4-methyl-1-piperazinyl)acetyl]-, labeled with tritium, (-)- (9CI) (CA INDEX NAME)



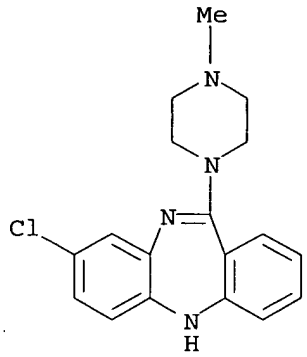
RN 122219-70-9 HCAPLUS
CN 10H-Thieno[3,4-b][1,5]benzodiazepin-10-one, 4,9-dihydro-3-methyl-4-[(4-methyl-1-piperazinyl)acetyl]-, labeled with tritium (9CI) (CA INDEX NAME)



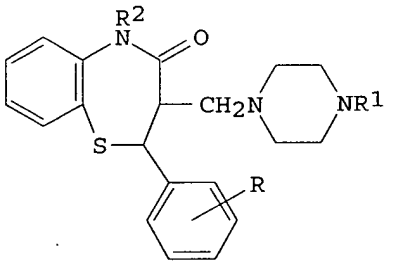
L95 ANSWER 25 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:135210 HCAPLUS
DOCUMENT NUMBER: 110:135210
TITLE: Synthesis of [3H]clozapine
AUTHOR(S): De Paulis, Tomas; Davis, Daniel A.; Smith, Howard E.; Malarek, David H.; Liebman, Arnold A.
CORPORATE SOURCE: Dep. Chem., Vanderbilt Univ., Nashville, TN, 37235, USA
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1988), 25(9), 1027-33
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:135210

AB [3H]clozapine was prepared with a specific activity of 9.9 Ci/mmol by reaction of 8-chloro-11-(methylthio)-5H-dibenzo[b,e][1,4]diazepine with an excess of [3H]N-methylpiperazine. The latter was prepared from N-methylpyrazinium bromide in ethanolic HCl by reduction at room temperature with tritium over 5% Rh on Al2O3.

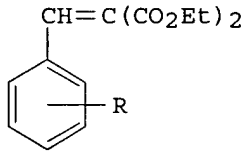
CC 28-21 (Heterocyclic Compounds (More Than One Hetero Atom))
IT 5786-21-0P, Clozapine **119550-28-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **119550-28-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 119550-28-6 HCAPLUS
CN 5H-Dibenzo[b,e][1,4]diazepine, 8-chloro-11-(4-methyl-1-piperazinyl)-, labeled with tritium (9CI) (CA INDEX NAME)



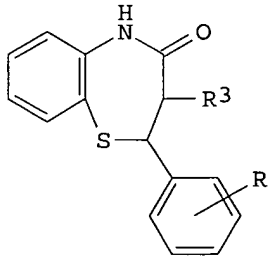
L95 ANSWER 26 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:630969 HCAPLUS
DOCUMENT NUMBER: 109:230969
TITLE: Synthesis of 2-aryl-2,3-dihydro-3-piperazinylmethyl-1,5-benzothiazepin-4(5H)-ones and related compounds
AUTHOR(S): Ohno, Sachio; Mizukoshi, Kiyoshi; Izumi, Kihachiro; Kato, Kazuo; Hori, Mikio
CORPORATE SOURCE: Res. Lab., Maruko Pharm. Co., Ltd., Kasugai, 486, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1988), 36(2), 551-62
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 109:230969
GI



I



II



III

AB A series of cis- and trans-piperazinylmethylbenzothiazepinones I [R = H, 3-Me, 3-Cl, 4-Me, 4-Cl, 4-OMe, 3,4-(OMe)2; R1 = H, Me, CH2CH2OH; R2 = Et,

Pr, Bu, PhCH2, allyl] were prepared Cyclocondensation of arylmethylenemalonates II with 2-HSC6H4NH2 gave benzothiazepinones III (R3 = CO2Et), which on reduction followed by mesylation or tosylation of the alcs. III (R3 = CH2OH), and coupling reactions with piperazinones gave I. Resolution of (±)-cis-I (R = R2 = H, R1 = H, Me) gave (-)-cis-I.

CC 28-22 (Heterocyclic Compounds (More Than One Hetero Atom))

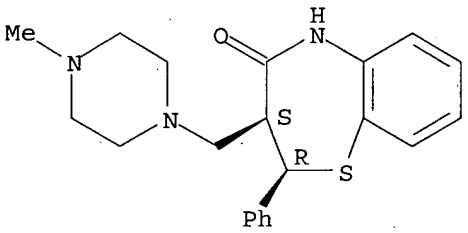
IT 109-01-3, N-Methylpiperazine 110-85-0, Piperazine, reactions **117553-64-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reactions of, with benzothiazepinones)

IT **117553-64-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reactions of, with benzothiazepinones)

RN 117553-64-7 HCAPLUS

CN 1,5-Benzothiazepin-4(5H)-one, 2,3-dihydro-3-[(4-methyl-1-piperazinyl)methyl]-2-phenyl-, labeled with deuterium, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L95 ANSWER 27 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1987:597467 HCAPLUS

DOCUMENT NUMBER: 107:197467

TITLE: Chemistry of nitrogen mustard [2-chloro-N-(2-chloroethyl)-N-methylethanamine] studied by nuclear magnetic resonance spectroscopy

AUTHOR(S): Golding, Bernard T.; Kebbell, Michael J.; Lockhart, Ian M.

CORPORATE SOURCE: Dep. Chem., University of Warwick, Coventry, CV4 7AL, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1987), (6), 705-13
CODEN: JCPKBH; ISSN: 0300-9580

DOCUMENT TYPE: Journal

LANGUAGE: English

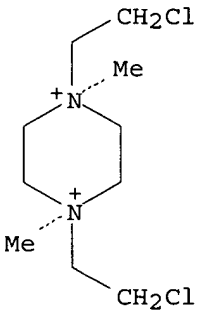
OTHER SOURCE(S): CASREACT 107:197467

AB MeN(CH2CH2X)2 (I; X = Cl) (II) was converted into the N-(2-chloroethyl)-N-methylaziridinium ion (III), which was characterized by NMR. Reactions of II with strong nucleophiles (e.g., S2O32-) gave disubstitution products (e.g., I; X = S2O3-). The intermediacy of III was inferred from the 13C distribution in product from 13C-labeled II. Less reactive nucleophiles (e.g., thiourea) yielded disubstitution products via spectroscopically detected intermediates III and ClCH2CH2NMeCH2CH2X [IV; e.g., X = SC+(NH2)2]. Weaker nucleophiles (e.g., guanosine) did not give substitution products. Reaction of II with NH3 gave a 3-2 ratio of I (X = NH2) and N-methylpiperazine (V). I (X = NH2) was formed from III, while V arose from intramol. cyclocondensation of IV (X = NH2).

CC 23-4 (Aliphatic Compounds)

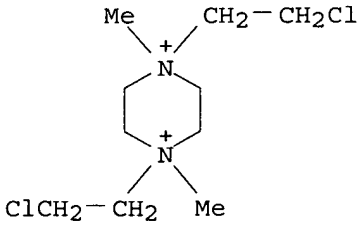
Section cross-reference(s): 22
IT 105-59-9P 109-01-3P, N-Methylpiperazine 1555-58-4P 4097-88-5P
37914-72-0P 98137-85-0P 111012-88-5P 111012-90-9P 111012-91-0P
111012-92-1P 111012-93-2P **111012-94-3P 111012-95-4P**
111012-96-5P 111012-97-6P 111012-98-7P 111012-99-8P 111036-16-9P
111036-17-0P 111036-18-1P 111036-19-2P 111036-21-6P 111068-26-9P
112023-61-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **111012-94-3P 111012-95-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 111012-94-3 HCAPLUS
CN Piperazinium, 1,4-bis(2-chloroethyl)-1,4-dimethyl-, labeled with carbon-13, dichloride, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



●2 Cl⁻

RN 111012-95-4 HCAPLUS
CN Piperazinium, 1,4-bis(2-chloroethyl)-1,4-dimethyl-, labeled with carbon-13, dichloride (9CI) (CA INDEX NAME)



●2 Cl⁻

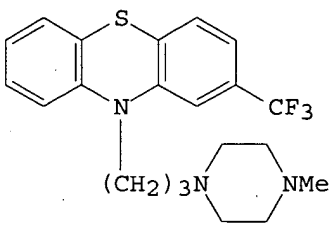
L95 ANSWER 28 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:17000 HCAPLUS
DOCUMENT NUMBER: 102:17000

TITLE: Radioimmunoassay for the sulfoxide metabolite of trifluoperazine and its application to a kinetic study in humans

AUTHOR(S): Aravagiri, M.; Hawes, E. M.; Midha, K. K.
CORPORATE SOURCE: Coll. Pharm., Univ. Saskatchewan, Saskatoon, SK, S7N 0W0, Can.

SOURCE: Journal of Pharmaceutical Sciences (1984), 73(10), 1383-7
CODEN: JPMSAE; ISSN: 0022-3549
DOCUMENT TYPE: Journal
LANGUAGE: English

GI



I

AB Antibodies were produced in rabbits immunized with 10[[3-[4-(2-carboxyethyl)-1-piperazinyl]-propyl]]-2-trifluoromethyl-10H-phenothiazine sulfoxide-bovine serum albumin conjugate. The subsequently developed radioimmunoassay (RIA) procedure enables, for the first time, the quantitation of the sulfoxide metabolite of trifluoperazine (I) [1549-88-8] in the plasma of humans after administration of therapeutic doses of trifluoperazine [117-89-5] in which 60 pg of the sulfoxide metabolite in 200 μL of plasma can be measured with a CV of <3%. Similar results were obtained by this assay with or without a benzene extraction step and also in the presence or absence of a large excess of trifluoperazine and suspected major metabolites of trifluoperazine. This RIA procedure, together with a previously developed RIA for trifluoperazine was used to directly determine plasma concns. of trifluoperazine and its sulfoxide metabolite after administration of a single, low, oral dose of trifluoperazine to 5 healthy volunteers. The rapidly appearing, relatively high concns. of the sulfoxide metabolite are indicative of presystemic sulfoxidn. The mean plasma elimination half-life for the sulfoxide metabolite of trifluoperazine was 5.8 h.

CC 1-1 (Pharmacology)

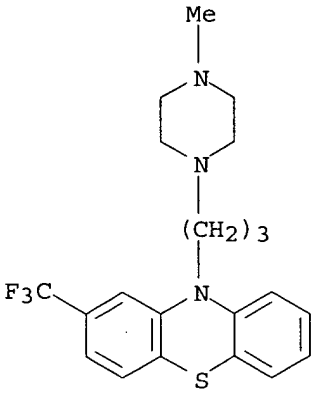
IT 41012-74-2 **93801-04-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of)

IT **93801-03-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

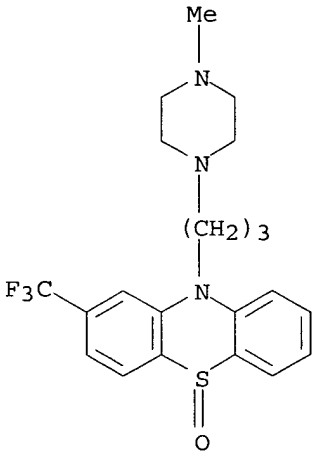
IT **93801-04-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of)

RN 93801-04-8 HCAPLUS

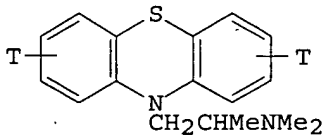
CN 10H-Phenothiazine, 10-[3-(4-methyl-1-piperazinyl)propyl]-2-(trifluoromethyl)-, labeled with tritium (9CI) (CA INDEX NAME)



IT **93801-03-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 93801-03-7 HCAPLUS
CN 10H-Phenothiazine, 10-[3-(4-methyl-1-piperazinyl)propyl]-2-(trifluoromethyl)-, 5-oxide, labeled with tritium (9CI) (CA INDEX NAME)



L95 ANSWER 29 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1982:492220 HCAPLUS
DOCUMENT NUMBER: 97:92220
TITLE: Tritium labeling of psychopharmacologic agents
AUTHOR(S): Buchman, Ouri; Shimoni, Michael
CORPORATE SOURCE: Radiochem. Dep., Nucl. Res. Cent. Negev, Beer Sheva, Israel
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1982), 19(1), 139-48
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Sixteen tritium-labeled phenothiazine tranquilizers were prepared with sp. activities of 10,000-40,000 mCi/mmol by bromination of phenothiazines with Br in AcOH or CHCl3 at room temperature followed by debromination-tritiation with T over 10% Pd/C in the presence of a large excess of Et3N. Tritiated promethazine (I) was obtained with a sp. activity of 36,700 mCi/mmol by sequential bromination and debromination of promethazine.

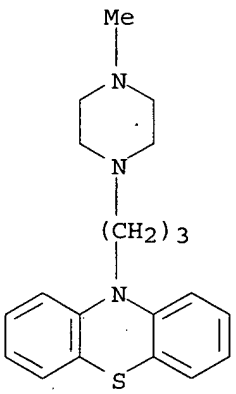
CC 28-14 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

IT 82353-92-2P 82353-93-3P 82353-94-4P 82353-95-5P 82353-96-6P
82353-97-7P **82353-98-8P** 82353-99-9P **82354-00-5P**
82354-01-6P 82354-02-7P 82354-03-8P **82354-04-9P**
82354-05-0P **82354-06-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **82353-98-8P 82354-00-5P 82354-04-9P**
82354-06-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

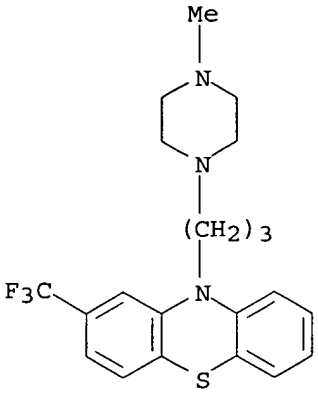
RN 82353-98-8 HCAPLUS

CN 10H-Phenothiazine-ar,ar-t2, 10-[3-(4-methyl-1-piperazinyl)propyl]- (9CI) (CA INDEX NAME)

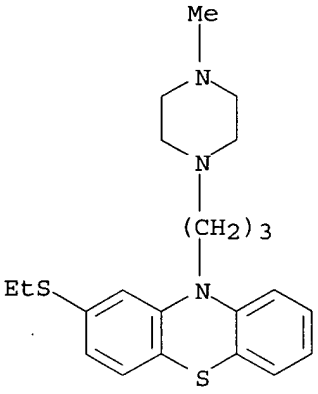


RN 82354-00-5 HCAPLUS

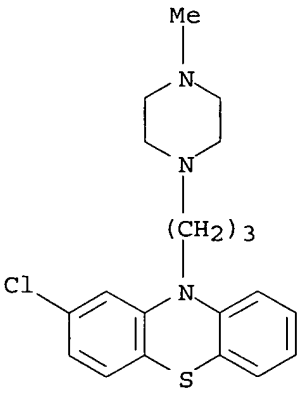
CN 10H-Phenothiazine-ar,ar-t2, 10-[3-(4-methyl-1-piperazinyl)propyl]-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 82354-04-9 HCAPLUS
CN 10H-Phenothiazine-ar,ar-t2, 2-(ethylthio)-10-[3-(4-methyl-1-piperazinyl)propyl]- (9CI) (CA INDEX NAME)



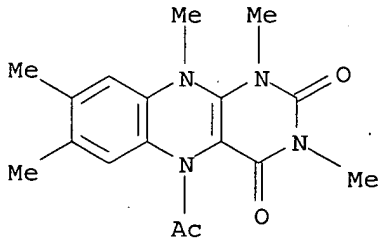
RN 82354-06-1 HCAPLUS
CN 10H-Phenothiazine-ar,ar-t2, 2-chloro-10-[3-(4-methyl-1-piperazinyl)propyl]- (9CI) (CA INDEX NAME)



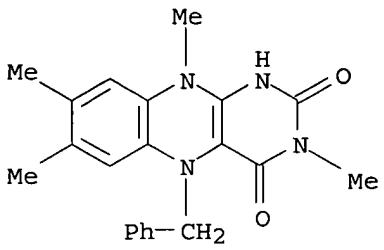
L95 ANSWER 30 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:134800 HCAPLUS
DOCUMENT NUMBER: 94:134800
TITLE: A comparative **carbon-13** NMR. Study on various reduced flavins
AUTHOR(S): Van Schagen, Cees G.; Mueller, Franz
CORPORATE SOURCE: Dep. Biochem., Agric. Univ., Wageningen, 6703 BC, Neth.
SOURCE: Helvetica Chimica Acta (1980), 63(8), 2187-201
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Various 2-electron reduced flavin derivs. were investigated by natural abundance 13C-NMR spectroscopy. Some selectively 13C-**enriched** compds. were synthesized to ensure the assignment of some of the quaternary C atoms of the flavin mol. Addition of 2 electrons to oxidized flavin leads to upfield shifts of all resonances except for those due to C(5a), C(9), and C(10'α). The largest upfield shift is observed for C(4a). Also some direct and 2-bond coupling consts. are reported. Theor. calcns. by INDO show that a rather good correlation exists between the calculated π-electron densities and the observed chemical shifts of the 2-electron reduced mol. For the oxidized mol., the correlation is less satisfactory. Most substitution effects are additive, but some deviations in some compds. are observed indicating structural differences between the compds. in question. The chemical shifts are also discussed in terms of the chemical reactivity of the oxidized and reduced flavin mol.

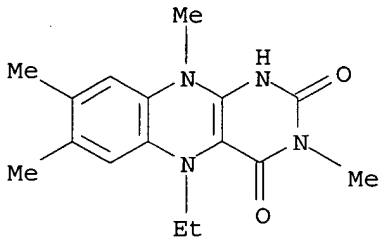
CC 7-3 (Enzymes)
IT Nuclear magnetic resonance
(of **carbon-13**, of reduced flavin)
IT **14453-92-0** 14453-97-5 **15578-97-9** 15578-98-0
21066-33-1 **50387-36-5 50387-38-7 53405-75-7**
58017-93-9 69447-57-0 77008-51-6 77008-52-7 77008-53-8
77008-54-9 77008-55-0 77008-56-1 **77008-57-2** 77012-50-1
RL: PRP (Properties)
(NMR of)
IT **14453-92-0 15578-97-9 50387-36-5**
50387-38-7 53405-75-7 77008-57-2
RL: PRP (Properties)
(NMR of)
RN 14453-92-0 HCAPLUS
CN Benzo[g]pteridine-2,4(1H,3H)-dione, 5-acetyl-5,10-dihydro-1,3,7,8,10-pentamethyl- (9CI) (CA INDEX NAME)



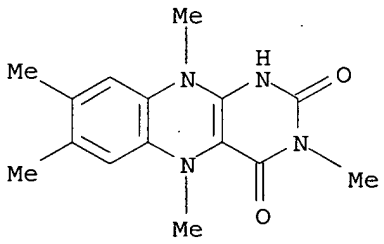
RN 15578-97-9 HCAPLUS
CN Benzo[g]pteridine-2,4(1H,3H)-dione, 5,10-dihydro-3,7,8-tetramethyl-5-(phenylmethyl)- (9CI) (CA INDEX NAME)



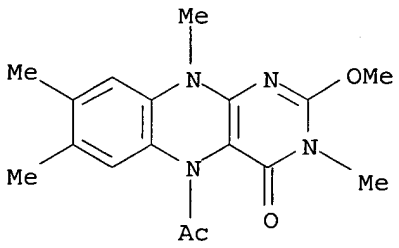
RN 50387-36-5 HCAPLUS
CN Benzo[g]pteridine-2,4(1H,3H)-dione, 5-ethyl-5,10-dihydro-3,7,8,10-tetramethyl- (9CI) (CA INDEX NAME)



RN 50387-38-7 HCAPLUS
CN Benzo[g]pteridine-2,4(1H,3H)-dione, 5,10-dihydro-3,5,7,8,10-pentamethyl- (9CI) (CA INDEX NAME)

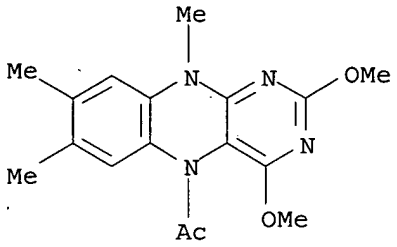


RN 53405-75-7 HCAPLUS
CN Benzo[g]pteridin-4(3H)-one, 5-acetyl-5,10-dihydro-2-methoxy-3,7,8,10-tetramethyl- (9CI) (CA INDEX NAME)



RN 77008-57-2 HCAPLUS

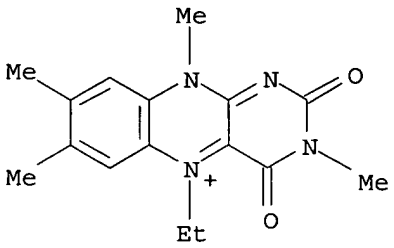
CN Benzo[g]pteridine, 5-acetyl-5,10-dihydro-2,4-dimethoxy-7,8,10-trimethyl- (9CI) (CA INDEX NAME)



L95 ANSWER 31 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:98615 HCAPLUS
DOCUMENT NUMBER: 94:98615
TITLE: NMR studies of 4a-**carbon-13**-**enriched** flavins with luciferase and other flavoproteins
AUTHOR(S): Lhoste, Jean Marc; Favaudon, Vincent; Ghisla, Sandro; Hastings, J. Woodland
CORPORATE SOURCE: Inst. Radium, Found. Curie, Orsay, Fr.
SOURCE: Flavins Flavoproteins, Proc. Int. Symp., 6th (1980), Meeting Date 1978, 131-8. Editor(s): Yagi, Kunio; Yamano, Toshio. Japan Sci. Soc. Press: Tokyo, Japan. CODEN: 44ECA6
DOCUMENT TYPE: Conference
LANGUAGE: English
AB 13C NMR data are presented for tetraacetylriboflavins, N(5)-deazariboflavins, and 3-methyl-4a,5-dihydrolumiflavin derivs. Assignments of 13C resonances were established on strong phys. and chemical grounds for the various ionic and redox states of isoalloxazine derivs. The 13C NMR spectra of the bacterial luciferase complex with FMN-4a-13C was also studied at low temps. in oxidized and dithionite-reduced systems. At low temps. the oxygenated intermediate formed on injection of O2 into the system was relatively stable, and the position of the O substituent at the 4a-C was confirmed.
CC 7-3 (Enzymes)
ST flavin **carbon 13** NMR; luciferase FMN NMR
IT Nuclear magnetic resonance
(of **carbon-13**, in flavins and FMN luciferase complex)
IT 752-13-6 15578-98-0 18717-85-6 19342-73-5 21066-33-1
37006-31-8 50387-29-6 63722-13-4 75621-98-6 75638-24-3
RL: PRP (Properties)
(**carbon-13** NMR of)
IT **37006-31-8**
RL: PRP (Properties)
(**carbon-13** NMR of)
RN 37006-31-8 HCAPLUS
CN Benzo[g]pteridinium, 5-ethyl-2,3,4,10-tetrahydro-3,7,8,10-tetramethyl-2,4-dioxo-, perchlorate (9CI) (CA INDEX NAME)

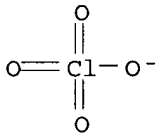
CM 1

CRN 47194-13-8
CMF C16 H19 N4 O2

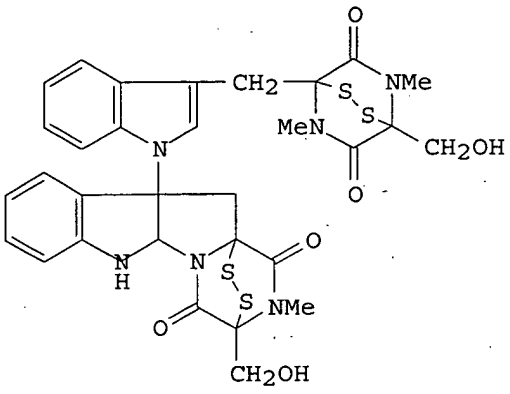


CM 2

CRN 14797-73-0
CMF Cl O4



L95 ANSWER 32 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1979:22988 HCAPLUS
DOCUMENT NUMBER: 90:22988
TITLE: Sporidesmins. Part 16. The structure of chetomin, a toxic metabolite of Chaetomium cochliodes, by **nitrogen-15** and **carbon-13** nuclear magnetic resonance spectroscopy
AUTHOR(S): Brewer, D.; McInnes, A. G.; Smith, D. G.; Taylor, A.; Walter, J. A.; Loosli, H. R.; Kis, Z. L.
CORPORATE SOURCE: Atlantic Reg. Lab., Natl. Res. Counc. Canada, Halifax, NS, Can.
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1978), (10), 1248-51
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Anal. of the 13C and 15N NMR spectra of chetomin (I), biosynthesized by C. cochliodes, showed that the sporidesmin-like and 3-(ω-skatyl)-3,6-epidithiopiperazine-2,5-dione **fragments** are linked by a bond between the indole N and the quaternary β-indoline C.

CC 28-22 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 10, 22

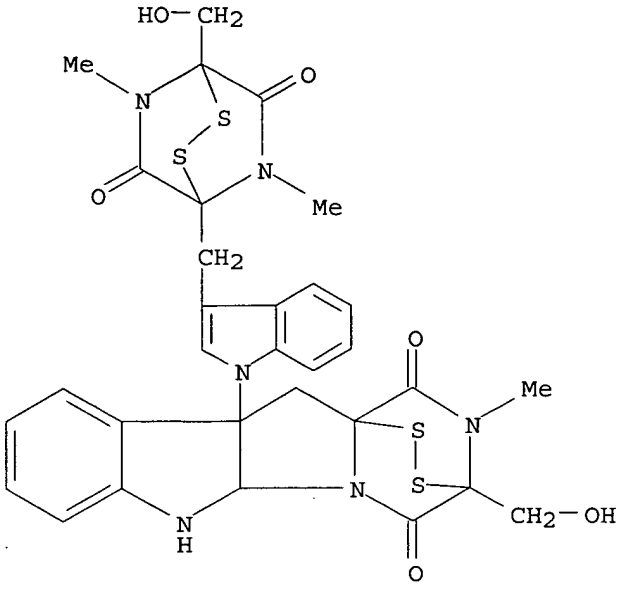
IT Nuclear magnetic resonance
(of **carbon-13** and **nitrogen-15**, in chetomin, structure in relation to)

IT **1403-36-7**
RL: PRP (Properties)
(mol. structure of, **carbon-13** and **nitrogen -15** NMR study of)

IT **1403-36-7**
RL: PRP (Properties)
(mol. structure of, **carbon-13** and **nitrogen -15** NMR study of)

RN 1403-36-7 HCAPLUS

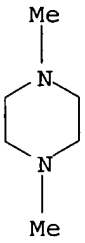
CN 3,11a-Epidithio-11aH-pyrazino[1',2':1,5]pyrrolo[2,3-b]indole-1,4-dione, 2,3,5a,6,10b,11-hexahydro-3-(hydroxymethyl)-10b-[(1S,4R)-3-[[4-(hydroxymethyl)-5,7-dimethyl-6,8-dioxo-2,3-dithia-5,7-diazabicyclo[2.2.2]oct-1-yl]methyl]-1H-indol-1-yl]-2-methyl-, (3S,5aR,10bS,11aS)- (9CI) (CA INDEX NAME)



L95 ANSWER 33 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1966:35193 HCAPLUS
DOCUMENT NUMBER: 64:35193
ORIGINAL REFERENCE NO.: 64:6454c-d
TITLE: J13C-H for substituted aldehydes
AUTHOR(S): Hammaker, R. M.
CORPORATE SOURCE: Kansas State Univ., Manhattan
SOURCE: Canadian Journal of Chemistry (1965), 43(10), 2916-18
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The equation of Malinowski (M., et al., CA 57, 11869g), J13C-H(XCHO) = J13C-H(HCHO) + 4/3[J13C-H(Me-X) -J13C-H(CH4)] (I), where X is a group of atoms, gives values which are different from the exptl. value. The difference, Δ = 0.658 J13C-H(XCHO), is necessary to have reliable results. This correction seems to be due to a neg. π-electron contribution to J13C-H. The correction increases linearly with the electronegativity of the first C-bonded atom of X and of the group electronegativity of X.

CC 32 (Physical Organic Chemistry)
IT Aldehydes
(**carbon-13** nuclear spin-spin coupling with H in)
IT 50-53-3, Phenothiazine, 2-chloro-10-[3-(dimethylamino)propyl]- 75-50-3, Trimethylamine **106-58-1**, Piperazine, 1,4-dimethyl- 108-01-0, Ethanol, 2-(dimethylamino)-
(detection of)
IT 14762-74-4, Carbon, **isotope** of mass 13
(nuclear spin-spin coupling with H in aldehydes)
IT **106-58-1**, Piperazine, 1,4-dimethyl-
(detection of)
RN 106-58-1 HCAPLUS
CN Piperazine, 1,4-dimethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



L95 ANSWER 34 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1955:12027 HCAPLUS
DOCUMENT NUMBER: 49:12027
ORIGINAL REFERENCE NO.: 49:2443a-f
TITLE: Synthesis of carbon14-labeled diethylcarbamazine, 1-diethylcarbamoyl-4-methylpiperazine
AUTHOR(S): Chase, B. H.; Downes, A. M.
CORPORATE SOURCE: Natl. Inst. Med. Research, London
SOURCE: Journal of the Chemical Society (1953) 3874-7
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 49:12027
GI For diagram(s), see printed CA Issue.
AB The introduction of 1-diethylcarbamoyl-4-methylpiperazine (I) has been a major advance in the treatment of filariasis. The synthesis of labeled material was undertaken to learn about the fate of the drug in the body. PhCH2N(CH2CO2H)2, m. 204°, was prepared in 50% yield by a method similar to that for MeN(CH2CO2H)2 [Organic Syn. Coll. Volume II, 397(1943)], and converted by hydrogenolysis over Pd-C to 88% HN(CH2CO2H)2, m. 232° (decomposition), which, refluxed with 40% HCHO and HCO2H, gave 95% MeN(CH2CO2H)2, m. 215-16° (decomposition). 1-Methyl-3,5-piperazinedione, m. 103-4°, was prepared by heating MeN(CH2CO2H)2 and urea in an open test tube (87% yield). 1-Methyl-2,5-piperazinedione, m. 141-3°, was prepared by refluxing a mixture of sarcosylglycine and (CH2OH)2. LiAlH4 reduction of either dione gave 1-methylpiperazine, isolated as the di-HCl salt monohydrate, m. 84-6°; after drying in vacuo over P2O5 at 100°, it m. 242-3°; dipicrate, m. 265°. Synthesis of labeled I: NH(C14H2CO2H)2 was isolated by chromatographing an aqueous solution of the residues (total activity 25.8 mc.; 6.56 mc. as iminodiacetic acid) from glycine-2-C14 prepns.; the total yield of HN(C14H2CO2H)2.HCl was 204.9 mg. [5.90 mc., specific activity, s.a. (in millicuries/millimole) 4.88]. The free acid was liberated with pyridine in absolute alc., filtered off after 2 hrs. at 0°, and 2 more crops were obtained by addition of inactive carrier HN(CH2CO2H)2 to the mother liquors, concentration of the solution, and precipitation with absolute alc.; total radio chemical yield was 5.49 mc. (93%). A portion of the HN(C14H2CO2H)2 was methylated with HCO2H and HCHO as described above (yield, 92%). The MeN(C14H2CO2H)2 (146.4 mg.; 2.93 mc.) heated with urea, formed MeN.C14H2.CO.NH.CO.C14H2 (76.8 mg.; 1.76 mc., s.a. 2.93), which was reduced with LiAlH4 in Et2O to 72% MeN.C14H2.CH2.NH.CH2C14H2.2HCl.H2O (II) (188.3 mg., 1.26 mc., s.a. 1.28). II treated with Et2NCOCl in NEt3 and CHCl3, the CHCl3 removed in a stream of dry air, the NEt3.HCl filtered off, washed, and the filtrate and washings concentrated to 5 cc. and treated with citric acid in Et2O gave 1-diethylcarbamoyl-4-methylpiperazine-3,5-C214 di-H citrate as an oil which solidified on scratching, yielding after

filtering, washing, and drying in vacuo, 179.9 mg. (0.58 mc., s.a. 1.27; 90%).

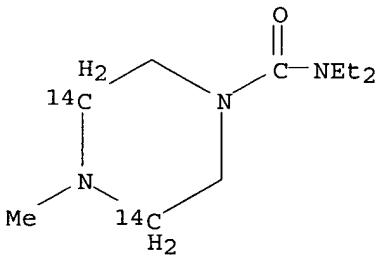
CC 10 (Organic Chemistry)

IT 142-73-4, Acetic acid, iminodi- 3987-53-9, Acetic acid, (benzylimino)di- 4408-64-4, Acetic acid, (methylimino)di- 5625-52-5, 2,5-Piperazinedione, 1-methyl- 60725-35-1, 2,6-Piperazinedione, 4-methyl- 856844-08-1, Piperazine-2,6-C142, 1-methyl- **856844-40-1**, 1-Piperazine-3,5-C142-carboxamide, N,N-diethyl-4-methyl- **856844-41-2**, 1-Piperazine-3,5-C142-carboxamide, N,N-diethyl-4-methyl-, citrate 856844-96-7, 2,6-Piperazinedione-3,5-C142, 4-methyl- 861067-49-4, Acetic-2-C14 acid, (methylimino)di- 861067-51-8, Acetic-2-C14 acid, iminodi-, hydrochloride 861067-52-9, Acetic-2-C14 acid, iminodi-
(preparation of)

IT **856844-40-1**, 1-Piperazine-3,5-C142-carboxamide, N,N-diethyl-4-methyl- **856844-41-2**, 1-Piperazine-3,5-C142-carboxamide, N,N-diethyl-4-methyl-, citrate
(preparation of)

RN 856844-40-1 HCAPLUS

CN 1-Piperazine-3,5-C142-carboxamide, N,N-diethyl-4-methyl- (5CI) (CA INDEX NAME)

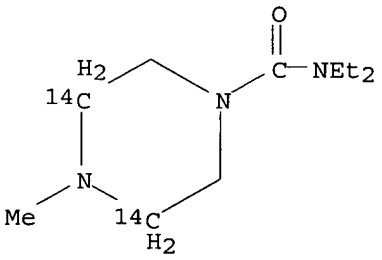


RN 856844-41-2 HCAPLUS

CN 1-Piperazine-3,5-C142-carboxamide, N,N-diethyl-4-methyl-, citrate (5CI) (CA INDEX NAME)

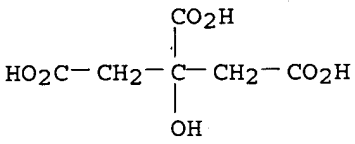
CM 1

CRN 856844-40-1
CMF C10 H21 N3 O



CM 2

CRN 77-92-9
CMF C6 H8 O7



L95 ANSWER 35 OF 37 USPATFULL on STN

ACCESSION NUMBER:	2005:177376 USPATFULL
TITLE:	Analysis of mass spectral data in the quiet zones
INVENTOR(S):	Pappin, Darryl J.C., Boxborough, MA, UNITED STATES
PATENT ASSIGNEE(S):	Applera Corporation, Framingham, MA, UNITED STATES (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2005153456	A1	20050714
APPLICATION INFO.:	US 2004-999638	A1	20041126 (10)

	NUMBER	DATE
PRIORITY INFORMATION:	US 2003-525478P	20031126 (60)
	US 2004-547375P	20040224 (60)

DOCUMENT TYPE:	Utility
FILE SEGMENT:	APPLICATION
LEGAL REPRESENTATIVE:	APPLIED BIOSYSTEMS, 500 OLD CONNECTICUT PATH, FRAMINGHAM, MA, 01701, US
NUMBER OF CLAIMS:	35
EXEMPLARY CLAIM:	1
NUMBER OF DRAWINGS:	6 Drawing Page(s)
LINE COUNT:	699

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Embodiments of this invention relate to the analysis of mass spectral data in the quiet zones.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

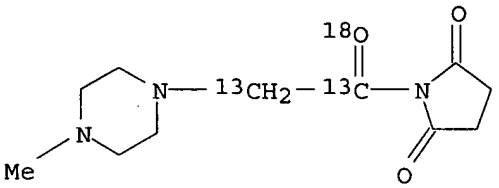
IT **853995-43-4 853995-44-5 853995-45-6 853995-46-7**
(anal. of mass spectral data in quiet zones using label fragment ions and applications in anal. of proteins and other biomols.)

IT **853995-47-8P 853995-48-9P 853995-49-0P 853995-50-3P**
(label fragment ion; anal. of mass spectral data in quiet zones using label fragment ions and applications in anal. of proteins and other biomols.)

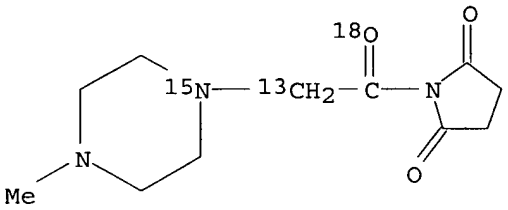
IT **853995-43-4 853995-44-5 853995-45-6 853995-46-7**
(anal. of mass spectral data in quiet zones using label fragment ions and applications in anal. of proteins and other biomols.)

RN 853995-43-4 USPATFULL

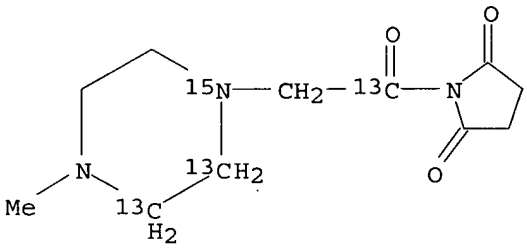
CN 2,5-Pyrrolidinedione, 1-[(4-methyl-1-piperazinyl)acetyl-13C2-18O]- (9CI) (CA INDEX NAME)



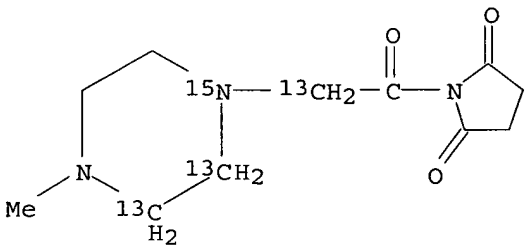
RN 853995-44-5 USPATFULL
CN 2,5-Pyrrolidinedione, 1-[(4-methyl-1-piperazinyl-1-15N)acetyl-2-13C-18O]- (9CI) (CA INDEX NAME)



RN 853995-45-6 USPATFULL
CN 2,5-Pyrrolidinedione, 1-[(4-methyl-1-piperazinyl-2,3-13C2-1-15N)acetyl-1-13C]- (9CI) (CA INDEX NAME)



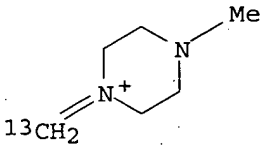
RN 853995-46-7 USPATFULL
CN 2,5-Pyrrolidinedione, 1-[(4-methyl-1-piperazinyl-2,3-13C2-1-15N)acetyl-2-13C]- (9CI) (CA INDEX NAME)



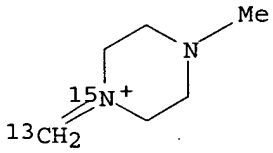
IT **853995-47-8P 853995-48-9P 853995-49-0P**
853995-50-3P
(label fragment ion; anal. of mass spectral data in quiet zones using

label fragment ions and applications in anal. of proteins and other biomols.)

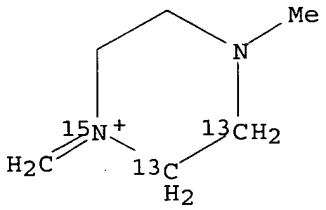
RN 853995-47-8 USPATFULL
CN Piperazinium, 4-methyl-1-(methylene-13C)- (9CI) (CA INDEX NAME)



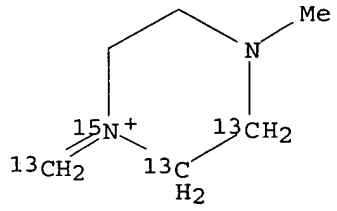
RN 853995-48-9 USPATFULL
CN Piperazinium-1-15N, 4-methyl-1-(methylene-13C)- (9CI) (CA INDEX NAME)



RN 853995-49-0 USPATFULL
CN Piperazinium-2,3-13C2-1-15N, 4-methyl-1-methylene- (9CI) (CA INDEX NAME)



RN 853995-50-3 USPATFULL
CN Piperazinium-2,3-13C2-1-15N, 4-methyl-1-(methylene-13C)- (9CI) (CA INDEX NAME)



L95 ANSWER 36 OF 37 USPATFULL on STN
ACCESSION NUMBER: 95:34186 USPATFULL
TITLE: Certain 1-methyl-piperidine-4-spiro-4'-(1'-3'-oxazolines) and corresponding -(1',3' thiazolines)
INVENTOR(S): Fisher, Abraham, Holon, Israel
Segall, Yoffi, Ramat Hasharon, Israel

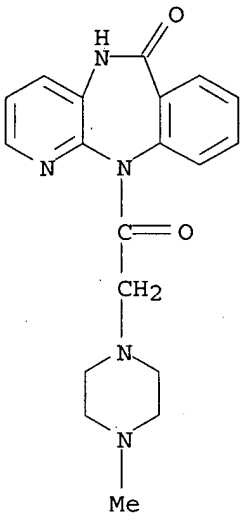
Shirin, Ezra, Tel Aviv, Israel
Karton, Yishai, Ness Ziona, Israel
Meshulam, Haim, Bat Yam, Israel
PATENT ASSIGNEE(S): Israel Institute for Biological Research, Ness Ziona, Israel (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 5407938		19950418
APPLICATION INFO.:	US 1993-137690		19931014 (8)

RELATED APPLN. INFO.: Continuation of Ser. No. US 1991-685397, filed on 9 Apr 1991, now abandoned which is a continuation-in-part of Ser. No. US 1990-507708, filed on 10 Apr 1990, now abandoned
DOCUMENT TYPE: Utility
FILE SEGMENT: Granted
PRIMARY EXAMINER: Rotman, Alan L.
LEGAL REPRESENTATIVE: Darby & Darby
NUMBER OF CLAIMS: 4
EXEMPLARY CLAIM: 1
LINE COUNT: 1356
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention relates to compounds (I) for treating diseases of the central and peripheral nervous system, including enantiomers, racemates and acid addition and quaternary salts, ##STR1## wherein Q is selected from two H atoms, (CH.sub.2).sub.m and C(CH.sub.3).sub.2 where m is 1, 2 or 3 and n and p are; each independently 0, 1, 2 or 3, provided that n+p=1-3, and R.sup.0 is H, methyl or OH; the moiety ##STR2## R is selected from H, NH.sub.2, NH-C.sub.1-6 -alkyl, N(C.sub.1-6 -alkyl).sub.2, C.sub.1-6 -alkyl, C.sub.2-6 -alkenyl, C.sub.2-6 -alkynyl, C.sub.3-7 - cycloalkyl, C.sub.1-6 -alkyl substituted by 1-6 halogen atoms, hydroxy- C.sub.1-6 -alkyl, C.sub.1-6 -alkoxy, C.sub.1-6 -alkylthio, C.sub.1-6 -alkoxy-C.sub.1-6 -alkyl, carboxy-C.sub.1-6 -alkyl, (C.sub.1-6 -alkoxy)carbonyl-C.sub.1-6 -alkyl, amino-C.sub.1-6 -alkyl, mono-(C.sub.1-6 -alkyl)amino-C.sub.1-6 -alkyl, di-(C.sub.1-6 -alkyl)amino-C.sub.1-6 -alkyl, 2-oxo-pyrrolidin-1-yl-methyl, aryl, diarylmethylol, and C.sub.1-6 -alkyl substituted by one or two aryl groups; R' is independently selected from the group from which R is selected and C.sub.1-6 -alkanoyl and arylcarbonyl; and aryl denotes unsubstituted phenyl or phenyl substituted by 1-3 substituents selected from halogen, C.sub.1-6 -alkyl, C.sub.1-6 -alkoxy and CF.sub.3, subject to certain provisos.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT 70761-70-5 **124620-97-9** 124620-98-0
(displacement from rat brain homogenate of, by spiro-oxathiolane/quinuclidine derivs.)
IT **124620-97-9**
(displacement from rat brain homogenate of, by spiro-oxathiolane/quinuclidine derivs.)
RN 124620-97-9 USPATFULL
CN 6H-Pyrido[2,3-b][1,4]benzodiazepin-6-one, 5,11-dihydro-11-[(4-methyl-1-piperazinyl)acetyl]-, labeled with tritium (9CI) (CA INDEX NAME)



L95 ANSWER 37 OF 37 USPATFULL on STN

ACCESSION NUMBER:	89:87547 USPATFULL
TITLE:	Oxathiolanes
INVENTOR(S):	Fisher, Abraham, Holon, Israel Karton, Ishai, Ness-Ziona, Israel
PATENT ASSIGNEE(S):	State of Israel, Israel Institute of Biological Research, Israel (non-U.S. government)

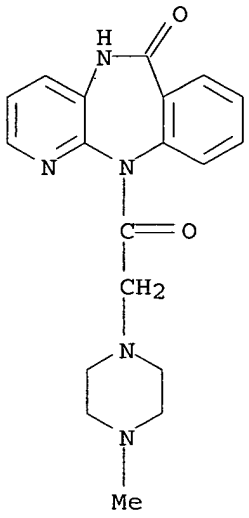
	NUMBER	KIND	DATE
PATENT INFORMATION:	US 4876260		19891024
APPLICATION INFO.:	US 1988-189210		19880502 (7)

RELATED APPLN. INFO.:	Continuation-in-part of Ser. No. US 1987-114473, filed on 28 Oct 1987, now abandoned
DOCUMENT TYPE:	Utility
FILE SEGMENT:	Granted
PRIMARY EXAMINER:	Bond, Robert T.
LEGAL REPRESENTATIVE:	Sheldon & Mak
NUMBER OF CLAIMS:	43
EXEMPLARY CLAIM:	1,9
LINE COUNT:	1306

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention accordingly provides in one aspect, novel spiro-oxathiolane/quinuclidine compounds corresponding with the schematic structural formula (I) ##STR1## and geometrical isomers, enantiomers, diastereoisomers, racemates and acid addition salts thereof, wherein one of Y and Z is 0 and the other is S(.dbd.O).sub.n ; n is 0, 1 or 2; R' and R" are each selected from the group consisting of hydrogen, alkyl, alkenyl, alkynyl, hydroxyalkyl, aminoalkyl, C.sub.3-7 cycloalkyl, aryl, diarylmethylol, and alkyl substituted by at least one aryl group, provided that at least R' and R" is other than hydrogen; and each X is hydrogen, or when Y is 0 and Z is S(.dbd.O).sub.n simultaneously, then each X may also be selected from the group consisting of deuterium and tritium, and provided further that when each X is hydrogen, Y is 0 and Z is S simultaneously, then at least one of R' and R" is selected from the group consisting of alkenyl, alkynyl, cyclopropyl, cyclobutyl, cycloheptyl, hydroxyalkyl and aminoalkyl.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT 70761-70-5 **124620-97-9** 124620-98-0
(displacement from rat brain homogenate of, by spiro-oxathiolane/quinuclidine derivs.)
IT **124620-97-9**
(displacement from rat brain homogenate of, by spiro-oxathiolane/quinuclidine derivs.)
RN 124620-97-9 USPATFULL
CN 6H-Pyrido[2,3-b][1,4]benzodiazepin-6-one, 5,11-dihydro-11-[(4-methyl-1-piperazinyl)acetyl]-, labeled with tritium (9CI) (CA INDEX NAME)



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